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(54) Title: UNDECAPRENYL PYROPHOSPHATE SYNTHASE (UPPS) ENZYME AND METHODS OF USE

UNDECAPRENYL PYROPHOSPHATE SYNTHASE (UPPS) ENZYME AND METHODS OF USE

Technical Field of the Invention

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The present invention relates generally to the identification of a novel undecaprenyl pyrophosphate synthase (herein "UPPS") crystalline structure. In addition, it provides a novel undecaprenyl pyrophosphate synthase active site of a crystalline structure in complex with Isopentenyl pyrophosphate and in complex with farnesyl pyrophosphate and methods to use these crystalline forms and their active sites to identify and improve undecaprenyl pyrophosphate synthase inhibitor compounds, among other uses. These compounds are characterized by the ability to competitively inhibit binding of substrates or other likemolecules to the active site of UPPS.

Background of the Invention

Polyisoprenoid molecules constitute a diverse and essential group of cellular polymers that function as sugar transporters, pigments, vitamins, hormones, etc. These molecules are products of a condensation of isopentenyl units that are produced by either of two pathways, a mevalonate-dependent or a mevalonate-independent pathway. IPP is a building block in the synthesis of squalene from which steroids are produced, and it is also a precursor of geranyl pyrophosphate from which polyisoprenols are synthesized (C. K. Mathews, and K. E. van Holde, 1996, Biochemistry). The successive condensation reactions to produce polyisoprenols from IPP are catalyzed by prenyltransferases of which there are at least 16 different enzyme forms in four distinct classes. These classes differ in the stereochemistry of the reaction they catalyze, the chain length of the substrates they use, and the chain length of their products. In the proposed two-step general mechanism of prenyltransferases, the first step is the elimination of the diphosphate from the allylic substrate, followed by the attack of the incoming IPP substrate to form a new carbon-carbon bond, followed by a stereospecific removal of a proton and formation of a new double bond (K. Ogura, and T. Koyama (1998) Chemical Reviews 98, 1263-1276; S. Ohnuma, T. Koyama, and K. Ogura (1989) FEBS Letters 257, 71-74).

In one of their many functions throughout the cell, polyisoprenol molecules are used as essential sugar carriers in the biosynthesis of glycoproteins in mammalian cells, and as essential sugar carriers in the biosynthesis of the bacterial cell wall. The peptidoglycan of the bacterial cell wall of Gram positive bacteria is formed by alternating units of N-acetylglucosamine, NAcGlc and N-acetylmuramic acid, NacMur. A pentapeptide chain with

sequence: (L-Ala)-(D-Glu)-(L-Lys)-(D-Ala)-(D-Ala) is linked through the N-terminal amino group of the peptide with the carboxyl group of the lactate moiety of NAcMur. These peptidoglycan chains are further cross-linked by connecting pentaglycine units. The NAcMur-pentapeptide is synthesized from UDP-NAcMur by successive additions of the corresponding amino acids catalyzed by various ligases, after which the NacMurpentapeptide is transferred to undecaprenolphosphate with the release of UMP. While linked to the undecaprenol carrier, NAcGlc and five glycine residues are added from Gly-tRNA. Subsequently, the NacGlc-NacMur-pentapeptide-pentaglycine intermediate is transferred to a peptidoglycan acceptor with the release of undecaprenyl pyrophosphate. In the next step, the terminal D-Ala is cleaved and released as adjacent peptidoglycan chains are cross-linked between the penultimate D-Ala of the first chain and the •-NH group of the lysine in the second chain. It is noteworthy that several molecules with antibacterial activity block various steps along this pathway. For example, bacitracin blocks the hydrolysis of the phosphodiester bond of undacaprenyl pyrophosphate to produce undecaprenylphosphate; vancomycin blocks the transfer of NacGlc-NacMur-pentapeptide-pentaglycine to the acceptor; and penicillin and cephalosporins block the transpeptidation, or cross-linking, between adjacent peptidoglycan chains.

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The sugar-carrier function of undecaprenolphosphate in bacteria is performed in mammalian cells by dolicholphosphate during N-linked glycosylation of peptides in the ER. 20 The human and bacterial homologous enzymes share about 34% amino acid sequence identity. Unlike undecaprenol, formed by 11 isopentenyl units, the dolichol molecule is nearly twice as large with 19-21 units. The amino acid sequence alignment of related UPPSs shows that contrary to other prenyl transferases, UPPS does not have the DDXXD sequence motif (A. Chen, P. A. Kroon, and C. D. Poulter (1994) Protein Science 3, 600-607). Instead, 25 several stretches of highly conserved residues are localized around a shallow cleft on the surface of the protein around the active site. This observation is consistent with the topology observed in the crystal structure of UPPS from Micrococcus luteus B-P 26, (M. Fujihashi, N. Shimizu, Y-W. Zhang, T. Koyama, and K. Miki (1999) Acta Crystallographica D55, 1606-1607; M. Fujihashi, Y-W. Zhang, Y. Higuchi, X-Y. Li, T. Koyama, and K. Miki 30 (2001) Proceedings of the National Academy of Sciences, U.S.A. 98, 4337-4342).

UPP is synthesized by the consecutive action of two enzymes: FPPS and UPPS. The crystal structure of FPPS in complex with FPP shows the FPP molecule bound in a deep pocket at a domain interface with a magnesium ion coordinated between the pyrophosphate and two aspartate residues in the DDXXD motif characteristic of these class of farnesyltransferases (L. C. Tarshis, M. Ynag, C. D. Poulter, and J. C. Sachettini (1994)

Biochemistry 33, 10871-10877). The FPPS product is an (all-E)-farnesyl diphosphate, one of the substrates for UPPS. UPPS is a (Z)-polyprenyldiphosphate synthase (prenyltransferase type IV) that catalyzes the sequential Z-addition of eight IPP molecules to an all-E-FPP to produce a E,Z-mixed-C55-isoprenyldiphosphate product, undecaprenyl pyrophosphate (M. Ito, M. Kobayashi, T. Koyama, and K. Ogura (1987) Biochemistry 26, 4745-4750):

UPPS, detergent,
$$Mg^{2+}$$

$$(all-E)\text{-FPP} + 8 \text{ IPP}$$

$$E,Z\text{-C}_{55}\text{-PP} + 8 \text{ PP}$$

The S. pneumoniae UPPS has a ${}^{FPP}_{K_{\mbox{\scriptsize m}}}$ of 0.5 μM and a ${}^{IPP}_{K_{\mbox{\scriptsize m}}}$ of 3.6 μM with a pH optimum of 7.5 - 8.0. The monomer has a pI of 5.1, a Mr • 29,000Da and is physiologically and catalytically active as a dimer. UPPS is an essential enzyme present in both Grampositive and Gram-negative pathogens, except in Mycoplasma (J. D. Mutle, and C. M. Allen (1989) Archives in Biochemistry and Biophysics 230, 49-60; I. Takahashi, and K. Ogura (1982) Journal of Biochemistry 92, 1527-1537; N. Shimizu, T. Kagawa, and K. Ogura (1998) Journal of Biological Chemistry 273, 19476-19481; C. M. Apfel, B. Takaca, M. Fountoulakis, M. Stieger, and W. Keck (1999) Journal of Bacteriology 181, 483-492).

The present invention provides a crystal structure of UPPS from Streptococcus 20 pneumoniae in its native state, and in complex with the substrates FPP and IPP. The structures show that UPPS is a dimer with an extensive contact area along a dimer interface. A shallow cleft harbors numerous conserved residues and delimits an active site. Several of these residues are disordered in a native enzyme but become well ordered in substratebound complexes. The crystal structures of the complexes with each of two substrates, FPP and IPP, provide a detailed description of these substrates' mode of binding, a structure of the Michaelis complex, certain critical residues involved in binding of substrates. The bound substrates and the residues that appear responsible for catalysis indicate a reaction mechanism, and map the available binding pockets used by inhibitors.

30 Summary of the Invention

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In one aspect, the invention provides a composition comprising a UPPS in crystalline form.

In another aspect, the present invention relates to a UPPS protein that is derived from Streptococcus pneumoniae comprising the amino acid sequence shown in SEQ ID No. 1 having coordinates of any or all of Tables I-III, said protein in an essentially pure native

form, or a homolog thereof. In a preferred embodiment, the invention provides a UPPS composition wherein said UPPS is a dimer.

In another aspect, the present invention provides a crystalline form of *Streptococcus* pneumoniae UPPS as derived from models of UPPS comprising coordinates of any or all of Tables I-III.

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In yet another aspect, the invention provides a UPPS protein in crystalline form having coordinates of Table IA, and interatomic distances and angles of active site residues listed in Table IIA and/or Table IIIA, respectively, in an essentially pure native form or a homolog thereof.

In yet another aspect, the invention provides a prenyltransferase of a *Streptococcus* pneumoniae UPPS in its native crystalline form. A preferred embodiment of the invention provides a prenyltransferase wherein said prenyltransferase has an active site formed by the amino acids Arg247, Gly250, Arg206, Arg200, Ser208, Tyr217, Asp28, Tyr70, Ile26, Phe72, Asn76, Met27, Ala71, particularly as ligands to IPP.

In yet another aspect, the invention provides a prenyltransferase wherein said prenyltransferase has an active site formed by the amino acids Asp28-Arg32, Arg79, Met27, His45, Gly48, Met49, Leu52, Ala71, Tyr70, Leu90, Pro91, Phe94, Phe149, particularly as ligands to FPP.

In another aspect, the invention provides a composition comprising a prenyltransferase in complex with FPP as characterized by the coordinates selected from the group consisting of the coordinates of Tables IB, and interatomic distances and angles of active site residues listed in IIB and/or IIIB.

In yet another aspect, the invention provides a composition comprising a prenyltransferase in complex with IPP as characterized by the coordinates selected from the group consisting of the coordinates of Tables IC, and interatomic distances and angles of active site residues listed in IIC and/or IIIC.

In another aspect, the invention provides a heavy atom derivative of a *Streptococcus* pneumoniae UPPS crystal wherein the prenyltransferase comprises a protein having the coordinates represented in any of Figures 2, 3, 4 and/or 5, and listed in Tables IA-IC, IIA-IIC, and/or IIIA-IIIC.

In another aspect, the invention provides a characterized by an $\alpha+\beta$ fold with three layers, $\alpha\beta\alpha$, wherein the β -strands form a six-strand parallel β -sheet and three α -helices pack against one face of the sheet and three to four α -helices located on the opposite face.

In yet another aspect, the invention provides a composition comprising a

Streptococcus pneumoniae UPPS in orthorhombic crystalline form having a space group of

 $P2_12_12_1$ wherin the lattice constants are a = 59.6Å, b = 118.0Å, c = 178.2Å and containing two 60 kDa dimers in an asymmetric unit.

In another aspect, the invention provides a composition comprising a *Streptococcus* pneumoniae UPPS in orthorhombic crystalline form having a space group of I2₁2₁2₁.

In yet another aspect, the invention provides a composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with IPP in orthorhombic crystalline form having a space group selected from the group consisting of P2₁2₁2₁ and I2₁2₁2.

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In yet another aspect, the invention provides a composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with a substrate FPP in monoclinic crystalline form having a space group of P2₁ and the crystalline form has lattice constants of a = 58.1 Å, b = 44.6 Å, c = 115.5 Å, $\beta = 98.7^{\circ}$.

In another aspect, the invention provides a process for determining a crystal structure form using structural coordinates of a *Streptococcus pneumoniae* UPPS crystal or portions thereof, to determine a crystal form of a mutant, homologue, or co-complex of said active site by molecular replacement.

In yet another aspect, the invention provides a process of identifying an inhibitor compound capable of binding to and inhibiting an enzymatic activity of a *Streptococcus pneumoniae* UPPS said process comprising: introducing into a suitable computer program information defining an active site conformation of a UPPS molecule comprising a conformation defined by coordinates listed in Table IA, IIA, and/or IIIA wherein said program displays the three-dimensional structure thereof; creating a three dimensional structure of a test compound in said computer program; displaying and superimposing a model of said test compound on a model of said active site; incorporating said test compound in a biological prenyltransferase activity assay for a prenyltransferase characterized by said active site; and determining whether said test compound inhibits enzymatic activity in said assay.

In another aspect, the invention provides a process designing drugs useful for inhibiting UPPS activity using certain or all of the atomic coordinates of a *Streptococcus* pneumoniae UPPS crystal to computationally evaluate a chemical entity for associating with an active site of a UPPS enzyme.

In yet another aspect, the invention provides a method of modifying a test UPPS polypeptide comprising: providing a test UPPS polypeptide sequence having a characteristic that is targeted for modification; aligning the test UPPS polypeptide sequence with at least one reference UPPS polypeptide sequence for which an X-ray structure or other structure is available, wherein the at least one reference UPPS polypeptide sequence has a characteristic

that is desired for the test UPPS polypeptide; building a three-dimensional model for the test UPPS polypeptide using the three-dimensional coordinates of the X-ray structure(s) or other structure(s) of the at least one reference UPPS polypeptide and its sequence alignment with the test UPPS polypeptide sequence; examining the three-dimensional model of the test UPPS polypeptide for a difference in an amino acid residue as compared to the at least one reference polypeptide, wherein the residues are associated with the desired characteristic; and mutating an amino acid residue in the test UPPS polypeptide sequence located at a difference identified to a residue associated with the desired characteristic, whereby the test UPPS polypeptide is modified.

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In another aspect, the invention provides a process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus pneumoniae* UPPS, said process comprising: carrying out an *in vitro* assay by introducing said compound in a biological prenyltransferase activity assay containing a prenyltransferase of the invention; and determining whether said test compound inhibits an enzymatic activity of the prenyltransferase in said assay.

In yet another aspect, the invention provides a product of the process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus* pneumoniae UPPS which is a peptide, peptidomimetic, or synthetic molecule and is useful for inhibiting the metallo-beta lactamase, preferably in the treatment of bacterial infections in a mammal.

In another aspect, the invention provides a product of the process of identifying an inhibitor compound capable of inhibiting an enzymatic activity of a *Streptococcus* pneumoniae UPPS wherein said product is a competitive or non-competitive inhibitor of the *Streptococcus* pneumoniae prenyltransferase.

In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS comprising using atomic coordinates of a Streptococcus pneumoniae UPPS crystal or atomic coordinates of a Streptococcus pneumoniae UPPS in complex with FPP or IPP to computationally evaluate a chemical entity for associating with an active site of a Streptococcus pneumoniae UPPS.

In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS comprising the step of using structure coordinates of Streptococcus pneumoniae UPPS to identify an intermediate in a chemical reaction between said prenyltransferase and a compound that is a substrate or inhibitor of said prenyltransferase. In another aspect, the invention provides a process of designing drugs useful for inhibiting Streptococcus pneumoniae UPPS wherein structure coordinates

comprise the coordinates corresponding to any of the structures shown in Figures 2, 3, 4 and/or 5 and/or listed in Tables IA-IC, IIA-IIC, and/or IIIA-IIIC.

In one aspect, the present invention relates to an UPPS that is derived from Streptococcus pneumoniae and comprising a protein having the amino acid sequence shown in SEQ ID No. 1, and coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II and/or III, in an essentially pure native form or a homolog thereof.

In another aspect, the present invention provides a novel crystalline form of a UPPS enzyme active site in complex with IPP, having the coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II, and/or III.

In yet another aspect, the present invention provides a novel crystalline form of the UPPS enzyme active site in complex with the substrate farnesyl pyrophosphate, identified herein FPP, having the coordinates of Table I, and interatomic distances and angles of active site residues listed in Table II, and/or III.

In yet another aspect, the invention provides a model of specific roles of residues in the active site responsible for the binding of substrates, substrate analogs, and inhibitors.

In yet another aspect, the invention provides astructural basis for the role of active site amino acid residues and metals bound in an active site in a catalytic activity of these enzymes. This aspect of the invention provides a method for identifying inhibitors of a UPPS, which methods comprise the steps of: providing coordinates of a UPP structure of the invention to a computerized modeling system; identifying compounds that bind to an active site; and screening the compounds identified for undecaprenyl pyrophosphate synthase inhibitory bio-activity.

Another aspect of this invention includes machine-readable media encoded with data representing coordinates of a three-dimensional structure of a UPPS crystal structure alone or in complex with IPP and/or FPP.

Other aspects and advantages of the present invention are described further in the following detailed description of the preferred embodiments thereof.

30 <u>Description of the Figures:</u>

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Figure 1A provides a representation of the chemical structure of FPP, and the numbering scheme used.

Figure 1B provides a representation of the chemical structure of IPP, and the numbering scheme used.

Figure 2A provides a representation of the secondary structure elements of native UPPS, from *Streptococcus pneumoniae*.

Figure 2B provides a representation of the topology of UPPS. Triangles denote β -strands and circles denote α -helices.

Figure 3A provides a schematic drawing of a UPPS enzyme from *Streptococcus* pneumoniae in complex with IPP bound in the active site.

Figure 3B provides a schematic drawing of a UPPS enzyme from *Streptococcus* pneumoniae in complex with FPP bound in the active site.

Figure 4A provides a schematic drawing of FPP bound in an active site of UPPS from S. pneumoniae. Shown and labeled in this view are the hydrophobic side chains of residues lining an FPP binding pocket, the interactions of the phosphate groups bound at the N-terminus of $\alpha 1$, a tightly bound water molecule, and the role of conserved arginine residues that are important for FPP binding.

Figure 4B provide a schematic drawing of FPP bound in the active site of UPPS from *S. pneumoniae*. In this view are shown, along the axis of the extended FPP molecule, the relative orientation of the important residues for catalysis, and those side chains important for substrate binding.

Figure 5 provides a schematic drawing of the interactions between the active site residues of a UPPS from *Streptococcus pneumoniae* and the substrate IPP. Important for the substrate binding are arginine side chains from the C-terminus of the other molecule in a dimer. Also shown is a pyrophosphate molecule that occupies the same position as the pyrophosphate moiety of FPP.

Detailed Description of the Invention

The present invention provides a *Streptococcus pneumoniae* UPPS crystalline structure of a native enzyme. In addition, it provides an undecaprenyl pyrophosphate synthase active site of the crystalline structure of the UPPS, in complex with IPP and in complex with FPP and methods to use these crystalline forms and their active sites to identify and improve UPPS inhibitor compounds (peptide, peptidomimetic or synthetic compositions). These compounds are characterized by an ability to competitively inhibit binding of substrates or other like-molecules to the active site of undecaprenyl pyrophosphate synthases.

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A UPPS from Streptococcus pneumoniae crystalline three-dimensional structure and its complex with IPP and FPP

The crystal structures of aUPPS from *Streptococcus pneumoniae* in its native form, in complex with the substrate IPP (Figure 1B), and a substrate, FPP (Figure 1A) have been determined and refined to 2.3Å, 2.8Å and 3.3Å resolution, respectively.

Native UPPS from Streptococcus pneumoniae crystalline structure was determined. This crystal structure consists of two homodimers in the asymmetric unit, molecules A and B form one active dimer, and molecules C and D form the second dimer. A preferred model includes residues 17-72 and 77-248 in molecule A; residues 17-72 and 79-246 in molecule B; residues 17-73 and 77-248 in molecule C; residues 18-73 and 78-246 in molecule D; and a total of 410 water molecules (Figure 2A). Each polypeptide chain has an • + • fold characterized by three layers: • • •. Four •-helices packed against one face of the central •sheet, formed by six parallel •-strands with ordering 342156. Another three •-helices located at the other side of the sheet form most of the dimer interface (Figure 2B). The central sheet is not continuous from one molecule to the other in the dimer, rather, the •sheets from each monomer form an angle of approximately 90°. In the dimer, the N- and the C-terminus of molecule B are located near a shallow groove formed in molecule A, the proposed location of the active site suggesting that the termini on one molecule contribute to the binding of substrates in the other molecule. This may explain the need for the enzyme to be a dimer if catalysis is to occur, and the extensive 1,650 Å² of buried surface area at the dimer interface involving $\alpha 5$, $\alpha 6$, and $\alpha 7$. The dimer interface include interactions between three pairs of charged side chains: Arg170NH2:Asp214OD2 (3.1Å), Arg226NE:Glu239OE2 (2.8Å), and Glu239OE2:Arg226NE (2.6Å). Also across the interface interact Tyr237OH and Asn229ND2 (3.1Å).

There are three buried charged residues: Glu152, Arg200, His22. E152 is at the N-terminus of α 5 and contacts Wat146 (2.9Å), Tyr147OH (2.6Å), Gln214OE1 (3.2Å), Phe184N (2.8Å), and Gln214OE1 (3.1Å). Arg200 is located at the C-terminus of β 5 contacting with Ser218 OG (2.7Å), Arg216O (2.9Å), Asp46OD2 (3.1Å), and Wat410 (2.8Å). His22 is makes H-bonds with Leu192O (2.6Å) and Thr68OG1 (2.9Å).

There are five relatively small, and empty internal cavities. One cavity is next to Arg200, a residue presumably located in the active site. This cavity is bound by atoms in residues Ile198, Ile199, Arg200, Leu20, Leu22, Tyr221 and Phe222. Two more cavities are located on either side of a-helix α3, one is lined by Leu90, Pro91, Phe94, Tyr95, Val99,

Ile109, Ala125, Leu126, Ala129, and Phe143. The cavity on the other side of $\alpha 3$ is lined by His45, Phe86, Met49, Leu90, Leu52, Asn30, Ala71, Met27, and Trp227. The presence of these two cavities suggests that the helix may be displaced upon substrate binding and for product release or membrane association. Another cavity is located C-terminal to $\alpha 6$ and a portion of $\beta 3$ (His187, Phe184, Glu110, Ile112, Asn142, Met111) along the groove on the side of $\alpha 5$. This groove probably accommodates the product. N-terminal to $\beta 5$ is the last cavity (Asp191, Leu192, Arg193, Asp194, Pro195, Asp196) that may allow the $\alpha 6$ - $\beta 5$ connection slide sideways or back and forth when the product is being processed during catalysis. No solvent molecules have been found occupying these cavities.

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In all four molecules in the asymmetric unit, residues 74-76 are disordered in a S. pneumoniae native UPPS structure, and residues in the immediate vicinity have higher B-factors than the average of the structure suggesting that these residues are highly mobile in the absence of ligands or substrates, and that they may be part of the active site. In addition, based on the alignment of UPPS amino acid sequences, the most conserved residues are located in the short α -helix α 1 (residues 28-32) and α 2- β 3 (residues 73-83), and in the β 5- α 7 (residues 200-214) loops suggesting that the active site is located at the top of the sheet in a shallow groove, next to the disordered region. As discussed below, the crystal structures of the UPPS complexes with the substrates FPP and IPP confirm the location of the active site, the critical role played by the conserved residues for substrate binding and their role in catalysis, and show that the disordered residues become ordered upon substrate binding.

The undecaprenyl pyrophosphate synthases from S. pneumoniae and M. luteus share a 37% amino acid sequence identity and the polypeptide have the same fold. Superposition of the $C\alpha$ atoms of the M. luteus and S. pneumoniae native UPPS crystal structures results in an overall root mean square, rms, deviation of 0.6\AA .

The present invention also provides a novel undecaprenyl pyrophosphate synthase crystalline structure based on the UPPS *Streptococcus pneumoniae* undecaprenyl pyrophosphate synthase in complex with the substrates IPP and FPP.

In the FPP complex, one FPP molecule is bound in the active site. However, in the IPP complex structure, two large, adjacent electron density peaks appear in the active site, the first one corresponds to a pyrophosphate onto which the pyrophosphate of FPP can be superimposed. The second electron density peak corresponds to an entire IPP molecule. In both complex structures, the major structural changes between the native and the substrate complex structures is the ordering of the polypeptide chain between residues 72-79, to form two turns of a 3₁₀ helix and the opening of the entrance to the long, narrow hydrophobic

pocket where FPP binds. In the IPP complex, the C-terminus of the other molecule in the dimer also becomes ordered to form part of the IPP binding site.

The interactions between the substrates and the enzyme are summarize as follows:

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- 1. There are at least two substrate-binding sites, at least one of each corresponding to each of the two substrates. The FPP's pyrophosphate binds at the N-terminus of •-helix •1 and the C-terminal end of strands •1 and •2. The farnesyl carbon chain runs across •2 and •3. The IPP's pyrophosphate binding site is located next to an FPP site and also runs across the top strands •1 and •2, but on the other side of the •-sheet. The phosphate group interacts with Arg247 located on the C-terminus of the partner molecule in the dimer
- 2. The farnesyl chain binds into a tunnel lined by Met49, Leu52, Ala71, Leu90, Pro91, Phe94, Leu126, Phe143, and Leu145.
- 3. The isopentenyl chain binds into a shallow depression lined by Ile26, the C• carbon of Asp28, Tyr70, and Phe72. The isopentenyl chain is then substantially or completely enclosed by the farnesyl chain bound adjacent to it and by the C-terminus of the partner molecule in the dimer. They are bound in such a way that the *re* face of an attacking carbon is poised for the reaction.
- 4. The position of the Mg^{+2} ions in a metal binding site may be indicated by a strong difference in an electron density peak modeled as a water molecule is located between the two pyrophosphate groups observed bound in the IPP complex.
- 5. The enzymatic turnover cycle starts with binding of FPP required for a subsequent binding of IPP. IPP binding must follow FPP because a binding interaction is with magnesium that is bridging the two pyrophosphates. Also, the carbon chain of FPP forms part of the IPP binding pocket. The orientation of C02 of IPP is such, that C1 of FPP is facing the *re* face of the double bond, ideal for the attack on C1. This is necessary, since the removal of a proton by Asp28 (or Arg200) occurs from the opposite side (on C9) to produce a Z-double bond.
 - 6. A preferred mechanism provides a critical role for His45, in •2, to promote cleavage of the pyrophosphate moiety from FPP by positioning the NE2 atom to polarize C1 in FPP, in analogy to a mechanism of thiamine phosphate synthase. Another preferred mechanism involves a metal-triggered carbocation formation. Once an FPP is bound, the binding of IPP and Mg+2 result in the formation of a carbocation analogously to a mechanism postulated for other prenyltransferases (i.e., farnesyl synthase, or aristolochene synthase). In addition to His45, Asn30 and/or Asp28, or Arg200 in •1 is putatively important for a stereochemically- specific removal of a proton to form a double bond. These residues occupy suitable relative positions for catalysis as deduced from a comparison of

complex structures. Asn30, Asp28 or Arg200 are poised to assist a stereochemical-specific proton abstraction from an incoming isopentenyl unit from C09. These residues are highly conserved among UPPSs from a variety of organisms. Of 27 aligned amino acid sequences including bacterial, archaebacteria and eukariotic UPPS's, the stretch FGHKA that includes Gly44 is absolutely conserved while His45 is present in all but two known sequences. In these two known sequences, a tyrosine replaces the histidine. In the same alignment, an amino acid stretch that includes Asp28, IMDGN, Asp28, Gly29 and Asn30 is absolutely conserved. Site-directed mutagenesis of some conserved residues of UPPS from E. coli (Pan, J-J., Yang, L.-W., and Liang, P-H. (2000) Biochemistry 39, 13856-13861) can now be rationally explained by the discoveries of the present invention. Mutation of Asp26 or Glu213 to alanine causes a 1000-fold drop in k_{cat}. In S. pneumoniae Asp28 is equivalent to E. coli's Asp26. In a preferred catalytic mechanism provided by the invention, Asp28/Asp26 plays a key role in formation of a double bond in the product after condensation step has occurred by removing a proton that would result in a cis (Z) configuration. A second important mutation involves Glu213, in S. pneumoniae Glu219 is equivalent to E. coli's Glu213. Glu219/Glu213 interacts with and helps to position Arg206 in aproper orientation to interact with IPP in an active site. Arg206 is an important residue for binding of IPP.

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Certain mechanisms of the invention take into account the binding of the product's chain when the product exceeds 20 carbons. A model of a C30 intermediate having the preferred stereochemistry (trans, trans, cis, cis, cis) bound at the FPP binding site in an active site UPPS shows that the chain beyond the first 15 carbon atoms can exit the protein into the solvent or, more likely, into a phospholipid membrane or detergent micell through a opening created between helices •2 and •3. Creation of an opening requires the movement of side chains of Met49 and Tyr98, torsion of the side chains is sufficient to open a channel through which a product may exit. There is also the possibility, as has been suggested, that a product may fold on itself several times inside an FPP binding channel, but there does not seem possible since there is not enough space to accommodate a long carbon chain. The final product exits the protein by either a "pull" action from the pyrophosphate end, or by a "pull" action from the opposite end, but that implies that the pyrophosphate is dragged along an FPP binding channel and out through an inter-helix space.

Table I provides the atomic coordinates of preferrednative and complex crystal structures of UPPS from *S. pneumoniae*. This preferred native model includes residues 37-92 and 97-268 in molecule A, 37-92 and 99-266 in molecule B, 37-93 and 97-268 in molecule C, 38-93 and 98-266 in molecule D, for the four molecules, A, B, C, and D, in the crystallographic asymmetric unit. The amino acid sequence of a UPPS from *S. pneumoniae*

is provided in SEQ ID No. 1. Table II provides the distances, in Å, between atoms within a 5.0Å radius in anactive site including bound substrates FPP and IPP. Table III provides the angles (°) between active site atoms at are within 4.0Å of substrate FPP or IPP.

Small variations in the atomic coordinates shown in Tables I - III will occur such as upon refinement of a crystal structure from a different crystal form that will result in a new set of coordinates. The deviation on Cα atoms from the present coordinate set is not expected to substantially exceed a rms of 2.5Å. Similarly, bond angles and bond lengths will usually vary within a small range (Engh, R. A., and Huber, R. (1991) Acta Crystallogr. A47, 392-400), however, the inter-atomic interactions in Tables I - III will remain constant, within the experimental error, as will the relative conformation and orientation or positioning of residues in an active site. The atomic coordinates of an active site residues, including bound substrates, are provided in Tables I-III.

Mutants and Derivatives

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Herein, the terms "a" and "an" mean "one or more" when used in this application, including the claims.

The invention further provides homologues, co-complexes, mutants and derivatives of the UPPS crystal structure of the invention.

The term "homologue" means a protein having at least 30% amino acid sequence identity with a functional domain of UPPS. Preferably the percentage identity will be 40, or 50%, more preferably 60 or 70% and most preferably 80 or 90%. A 95% identity is most particularly preferred.

The term "co-complex" means a UPPS or a mutant or homologue of a UPPS in covalent or non-covalent association with a chemical entity or compound.

As used herein, the term "agonist" means an agent that supplements or potentiates the bioactivity of a functional UPPS gene or protein or of a polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. By way of specific example, an "agonist" is a compound that interacts with a steroid hormone receptor to promote a transcriptional response. An agonist can induce changes in a receptor that places a receptor in an active conformation that allows them to influence transcription, either positively or negatively. There can be several different ligand-induced changes in a receptor's conformation. The term "agonist" specifically encompasses partial agonists.

As used herein, the terms "•-helix", "alpha-helix" and "alpha helix" are used interchangeably and mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed

direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turnoff the helix, which extends about 0.56 nm along the long axis.

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As used herein, the term "antagonist" means an agent that decreases or inhibits a bioactivity of a functional UPPS gene or protein, or that supplements or potentiates a bioactivity of a naturally occurring or engineered non-functional UPPS gene or protein. Alternatively, an antagonist can decrease or inhibit a bioactivity of a functional gene or polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. An antagonist can also supplement or potentiate the bioactivity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a UPPS polypeptide. By way of specific example, an "antagonist" is a compound that interacts with a steroid hormone receptor to inhibit a transcriptional response. An antagonist can bind to a receptor but fail to induce conformational changes that alter a receptor's transcriptional regulatory properties or physiologically relevant conformations. Binding of an antagonist can also block the binding and therefore the actions of an agonist. The term "antagonist" specifically encompasses partial antagonists.

As used herein, the terms "•-sheet", "beta-sheet" and "beta sheet" are used interchangeably and mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the term "binding pocket" refers to any moiety, part or region of UPPS that actually or is capable of binding to, directly participating with, adhering to, or otherwise associating with an atom, ion or molecule. Preferably, a large cavity within a UPPS ligand binding domain where an agonist or antagonist can bind is a binding pocket. Such a cavity can be empty, or can contain water molecules or other molecules from the solvent, or an agonist or antagonist moieties, atoms or molecules. Such a binding pocket also includes regions of space near the "main" binding pocket that are not occupied by atoms or moieties of UPPS, but that are near the "main" binding pocket, and that are contiguous with the "main" binding pocket. Preferably,

As used herein, the term "active site" refers to a specific region of UPPS binding pocket where a molecule binds and catalysis takes place. It is comprised and bound by amino acid residues that are in direct contact with the substrate or that interact with the substrate(s) through water molecules or those amino acids that, although not being in direct contact with the substarte(s), nonetheless are important for they allow the correct

positioning of those amino acids that are and which without the correct positioning they would not be able to interact favorably (i. e. in a way conducent to catalysis) with the substrate(s). These interactions between amino acids and substrate(s) are responsible for the binding of the substrate to UPPS, for the correct positioning of the substrate for catalysis, and for stabilization of any reaction intermediates and for the binding and possibly the release of the products from that active site. These are amino acids that may be replaced by site-directed mutagenesis, and their replacement will result in at the very least a severalfold, or more likely, in several orders of magnitude decrease in the binding affinity of the substrate(s). The active site is also comprised by amino acids that are directly responsible for catalysis. These amino acids interact with the substrate(s) through hydrogen bonds or are in close proximity to electron-donor or electron-acceptor centers in the substrate. These amino acids may act themselves as electron-donor or electron-acceptor centers for catalysis to take place. These are amino acids that may be replaced by site-directed mutagenesis, and their replacement will result in at the very least a several-fold, or more likely, in several orders of magnitude decrease in the catalytic efficiency, but no changes in the affinity of binding of the substarte(s). In some cases, the catalytic activity may be recovered by some chemicals that, by binding to the appropriate active site residues, will mimic the wild-type amino acid.

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As used herein, the term "biological activity" means any observable effect flowing from interaction between a UPPS polypeptide and an agonist or antagonist. Representative, but non-limiting, examples of biological activity in the context of the present invention include transcription regulation, agonist or antagonist binding, and peptide binding.

As used herein, the terms "candidate substance" and "candidate compound" are used interchangeably and refer to a substance that is believed to interact with another moiety, for example an agonist or antagonist that is believed to interact with a complete, or a fragment of, a UPPS polypeptide, and which can be subsequently evaluated for such an interaction. Representative candidate substances or compounds include xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as glucocorticosteroids, steroids, fatty acids and prostaglandins. Other examples of candidate compounds that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a UPPS polypeptide, toxins and venoms, viral epitopes, hormones (e.g., glucocorticosteroids, opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

As used herein, the terms "cells," "host cells" or "recombinant host cells" are used interchangeably and mean not only to a particular subject cell, but also to any progeny or potential progeny of such a cell. Because certain modifications can occur in succeeding generations due to either mutation or environmental influences, such progeny might not, in fact, be identical to the parent cell, but are still included within the scope of the term as used herein.

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As used herein, the terms "chimeric protein" or "fusion protein" are used interchangeably and mean a fusion of a first amino acid sequence encoding a UPPS polypeptide with a second amino acid sequence defining a polypeptide domain foreign to, and not homologous with, any domain of a UPPS polypeptide. A chimeric protein can include a foreign domain that is found in an organism that also expresses the first protein, or it can be an "interspecies" or "intergenic" fusion of protein structures expressed by different kinds of organisms. In general, a fusion protein can be represented by the general formula X—UPPS—Y, wherein UPPS represents a portion of the protein which is derived from a UPPS polypeptide, and X and Y are independently absent or represent amino acid sequences which are not related to a UPPS sequence in an organism, which includes naturally occurring mutants.

As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

As used herein, the term "DNA segment" means a DNA molecule that has been isolated free of total genomic DNA of a particular species. In a preferred embodiment, a DNA segment encoding a UPPS polypeptide refers to a DNA segment that comprises any of SEQ ID NO:1, but can optionally comprise fewer or additional nucleic acids, yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Streptococcus pnuemoniae*. Included within the term "DNA segment" are DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

As used herein, the term "DNA sequence encoding a UPPS polypeptide" can refer to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in amino acid sequence of the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes

can be identical or can have certain modifications, including nucleotide substitutions, additions or deletions, all of which still code for polypeptides having substantially the same activity.

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced.

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As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences. Preferred embodiments of genomic and cDNA sequences are disclosed herein.

As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

As used herein, "hexagonal unit cell" means a unit cell wherein $a = b \cdot c$; and $\cdot = \cdot$ = 90, $\cdot = 120^{\circ}$. The vectors a, b, and c describe the unit cell edges and the angles \cdot , \cdot , and \cdot describe the unit cell angles. In a preferred embodiment of the present invention, the unit cell has lattice constants of a = 59.6Å, b = 118.0Å, c = 178.2Å. While preferred lattice constants are provided, a crystalline polypeptide of the present invention also comprises variations from the preferred lattice constants, wherein the variations range from about one to about two percent.

As used herein, the term "hybridization" means the binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

As used herein, the term "interact" means detectable interactions between molecules, such as can be detected using, for example, a yeast two hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions can, for example, be protein-protein or protein-nucleic acid in nature.

As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

As used herein, the term "modified" means an alteration from an entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant UPPS polypeptide, preferably a wild-type or mutant UPPS polypeptide. The term "modulation" as used herein refers to both up-regulation (i.e., activation or stimulation) and down-regulation (i.e. inhibition or suppression) of a response, and includes responses that are upregulated in one cell type or tissue, and down-regulated in another cell type or tissue.

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As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of a wild-type UPPS ligand binding domain, or a UPPS mutant crystal whose structure coordinates are unknown, by orienting and positioning a molecule or model whose structure coordinates are known within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. See, e.g., Lattman, (1985) Method Enzymol., 115: 55-77; Rossmann, ed, (1972) The Molecular Replacement Method, Gordon & Breach, New York. Using the structure coordinates of the active site of UPPS provided by this invention, molecular replacement can be used to determine the structure coordinates of a crystalline mutant or homologue of the UPPS active site, or of a different crystal form of the UPPS active site.

As used herein, the term "partial agonist" means an entity that can bind to a receptor and induce only part of the changes in the receptors that are induced by agonists. The differences can be qualitative or quantitative. Thus, a partial agonist can induce some of the conformation changes induced by agonists, but not others, or it can only induce certain changes to a limited extent.

As used herein, the term "partial antagonist" means an entity that can bind to a receptor and inhibit only part of the changes in the receptors that are induced by antagonists. The differences can be qualitative or quantitative. Thus, a partial antagonist can inhibit some of the conformation changes induced by an antagonist, but not others, or it can inhibit certain changes to a limited extent.

As used herein, the term "polypeptide" means any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides, and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides and proteins, unless otherwise noted. As used

herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product.

As used herein, the term "primer" means a sequence comprising two or more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

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As used herein, the term "sequencing" means the determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

As used herein, the terms "structure coordinates" and "structural coordinates" mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of coordinates determined by X-ray crystallography is not without standard error. In general, the error in the coordinates tends to be reduced as the resolution is increased, since more experimental diffraction data is available for the model fitting and refinement. Thus, for example, more diffraction data can be collected from a crystal that diffracts to a resolution of 2.8 angstroms than from a crystal that diffracts to a lower resolution, such as 3.5 angstroms. Consequently, the refined structural coordinates will usually be more accurate when fitted and refined using data from a crystal that diffracts to higher resolution. The design of agonists, antagonists, and modulators for UPPS depends on the accuracy of the structural coordinates. If the coordinates are not sufficiently accurate, then the design process will be ineffective. In most cases, it is very difficult or impossible to collect sufficient diffraction data to define atomic coordinates precisely when the crystals diffract to a resolution of only 3.5 angstroms or poorer. Thus, in most cases, it is difficult to use X-ray structures in structure-based agonist and antagonist design when the X-ray structures are based on crystals that diffract to a resolution of only 3.5 angstroms or poorer. However, common experience has shown that crystals diffracting to 2.8 angstroms or better can yield X-ray structures with sufficient accuracy to greatly facilitate structure-based drug design. Further improvement in the resolution can further facilitate structure-based design, but the coordinates obtained at 2.8 angstroms resolution are generally adequate for most purposes.

Also, those of skill in the art will understand that UPPS proteins can adopt different

conformations when different agonists, antagonists, and modulators are bound. Subtle variations in the conformation can also occur when different agonists are bound, and when different antagonists are bound. These variations can be difficult or impossible to predict from a single X-ray structure. Generally, structure-based design of UPPS modulators depends to some degree on a knowledge of the differences in conformation that occur when agonists and antagonists are bound. Thus, structure-based modulator design is most facilitated by the availability of X-ray structures of complexes with potent agonists as well as potent antagonists.

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As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which is it associated in nature.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to the following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to such gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

As used herein, the term "unit cell" means a basic parallelipiped shaped block. The entire volume of a crystal can be constructed by regular assembly of such blocks. Each unit

cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles •, •, and • define the angles between the vectors: angle • is the angle between vectors b and c; angle • is the angle between vectors a and c; and angle • is the angle between vectors a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

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As used herein, the term "mutant" or "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art. For example, a UPPS polypeptide, i.e., a polypeptide displaying the biological activity of wild-type UPPS activity, characterized by the replacement of at least one active-site amino acid from the wild-type prenyltransferase sequence. Such a mutant may be prepared, for example, by expression of the UPPS prenyltransferase cDNA previously altered in its coding sequence by oligonucleotide-directed mutagenesis.

UPPS mutants may also be generated by site-specific incorporation of unnatural amino acids into the UPPS protein using the general biosynthetic method of C. J. Noren et al, *Science*, 244:182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type UPPS is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis. A suppressor directed against this codon is then chemically aminoacylated *in vitro* with the desired unnatural amino acid. The aminoacylated residue is then added to an *in vitro* translation system to yield a mutant UPPS enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant metallo UPPS prenyltransferase by expression of UPPS-encoding cDNAs in auxotrophic *E. coli* strains (W. A. Hendrickson et al, *EMBO J.*, 9(5):1665-1672 (1990)) or a normal strain grown in a medium supplemented with appropriate nutrients that will prevent endogenous synthesis of methionine. In either of these methods, the wild-type or mutated undecaprenyl pyrophosphate synthase cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "heavy atom derivative" refers to derivatives of UPPS produced by chemically modifying a crystal of UPPS. In practice, a native crystal is tretaed by

immersing it in a solution containing the desired metal salt, or organometallic compound, e.g., lead chloride, gold thiomalate, thimerosal or uranyl acetate, which upon diffusion into the protein crystal can bind to the protein. The location of the bound heavy metal atom site(s) can be determined by X-ray diffraction analysis of the treated crystal. This information, in turn, is used to generate the phase angle information needed to construct a three-dimensional electron density map from which a model of the atomic structure of the enzyme is derived (T. L. Blundel and N. L. Johnson, *Protein Crystallography*, Academic Press (1976)).

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The term "space group" refers to the arrangement of symmetry elements (i.e. molecules) throughout the crystal. There are only 132 possible arrangements, each one unique and identified by a symbol. The space group symbol is formed by a letter (P, F, I, C) and numbers with or without subscripts, for example: P2₁, I222, C2₁2₁2₁, etc.

Methods of Identifying Inhibitors of UPPS from Streptococcus pneumoniae Crystalline Structure

An aspect of this invention involves a method for identifying inhibitors of a UPPS characterized by the crystal structure and novel active site described herein, and the crystal structures of the complexes with its substrates. The novel prenyltransferase crystalline structure of the invention permits the identification of inhibitors of prenyltransferase activity. Such inhibitors may be competitive, binding to all or a portion of the active site of UPPS; or non-competitive and bind to and inhibit undecaprenyl pyrophosphate synthase whether or not it is bound to another chemical entity.

One design approach is to probe a UPPS crystal of the invention with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate UPPS inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule binds. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for a UPPS inhibitor activity (J. Travis, *Science*, 262:1374 (1993)).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to or with a UPPS. Thus, the time-dependent analysis of structural changes in a UPPS during its interaction with other molecules is permitted. The reaction intermediates of the UPPS can also be deduced from the reaction product in co-complex with a UPPS. Such information is useful to design improved analogues of known UPPS inhibitors or to design

novel classes of inhibitors based on the reaction intermediates of a UPPS enzyme and UPPS inhibitor co-complex. This provides a novel route for designing UPPS inhibitors with both high specificity and stability.

Another approach made possible by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to a UPPS enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy (E. C. Meng et al, *J. Comp. Chem.*, 13:505-524 (1992)).

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Because UPPS may crystallize in more than one crystal form, the structure coordinates of UPPS, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of UPPS. They may also be used to solve the structure of UPPS mutant co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of UPPS.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of UPPS, a UPPS mutant, a UPPS co-complex, a UPPS from a different bacterial species, or the crystal of some other protein with significant amino acid sequence homology to any domain of UPPS, may be determined using the UPPS structure coordinates of this invention as provided in Figures 1-5 and Tables I - III. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Thus, preferred UPPS structures provided herein permits the screening of known molecules and/or the designing of new molecules which bind to the structure, particularly at the binding pocket or active site, via the use of computerized evaluation systems. For example, computer modeling systems are available in which the sequence of a UPPS, and a UPPS structure (i.e., the atomic coordinates, bond distances between atoms in the active site region, etc. as provided by Tables I - III herein) may be input. Thus, a machine readable medium may be encoded with data representing the coordinates of Tables I - III. The computer then generates structural details of the site into which a test compound should bind, thereby enabling the determination of the complementary structural details of said test compound.

More particularly, the design of compounds that bind to or inhibit UPPS according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with UPPS. Non-covalent molecular

interactions important in the association of UPPS with its substrate include hydrogen bonding, van der Waals, and hydrophobic interactions.

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Second, the compound must be able to assume a conformation that allows it to associate with UPPS. Although certain portions of the compound will not directly participate in this association with UPPS, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., binding pocket, active site, or substrate binding sites of UPPS, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with UPPS.

Another approach made possible by this invention is to screen computationally small molecule databases for chemical entities or compounds that can bind in whole, or in part, to a UPPS enzyme. Details on this process and the results it can provide are now documented in the art. For a description of this type of technology please refer to PCT application WO 97/16177 published 09 May 1997; the techniques described there for computer modeling are incorporated herein by reference.

Once identified by the modeling techniques, the prenyltransferase inhibitor may be tested for bio-activity using standard techniques. For example, the structure of the invention may be used in enzymatic activity assays to determine the inhibitory activity of the compounds or binding assays using conventional formats to screen inhibitors. One particularly suitable assay format includes the enzyme-linked immunosorbent assay (herein "ELISA"). Other assay formats may be used; these assay formats are not a limitation on the present invention.

The potential inhibitory or binding effect of a chemical compound on UPPS may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and UPPS, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to UPPS and inhibit using a suitable assay. In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of UPPS may be computationally evaluated and designed by means of a series of steps in that chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of UPPS.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with UPPS and more particularly with the individual binding pockets of the UPPS active site or accessory binding site. This process may begin by visual inspection of, for example, the active site on the computer screen based on the UPPS coordinates in Tables I-III. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an binding pocket or active site of UPPS. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

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Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

- 1. GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules", *J. Med. Chem.*, 28:849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
- MCSS (A. Miranker and M. Karplus, "Functionality Maps of Binding Sites:
 A Multiple Copy Simultaneous Search Method", Proteins: Structure, Function and Genetics, 11:29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, MA.
- 3. AUTODOCK (D. S. Goodsell and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing", *Proteins: Structure, Function, and Genetics*, 8:195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, CA.
 - 4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161:269-288 (1982)). DOCK is available from University of California, San Francisco, CA.

In addition, other commercially available computer databases for small molecular compounds includes Cambridge Structural Database, Fine Chemical Database, and CONCORD, for a review see Rusinko, A., Chem. Des. Auto. News 8, 44-47 (1993).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of UPPS. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems", Speical Pub., Royal Chem. Soc. 78, pp. 182-196 (1989)]. CAVEAT is available from the University of California, Berkeley, CA.

- 5 2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design," J. Med. Chem., 35:2145-2154 (1992).
- HOOK (available from Molecular Simulations, Burlington, MA).
 Instead of proceeding to build a UPPS inhibitor in a step-wise fashion one fragment
 or chemical entity at a time as described above, inhibitory or other UPPS binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known ligand(s). These methods include:
 - 1. LUDI (H.J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", *J. Comp. Aid. Molec. Design*, <u>6</u>:61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, CA.
 - 2. LEGEND (Y. Nishibata and A. Itai, *Tetrahedron*, 47:8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, MA.

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3. LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modelling techniques may also be employed in accordance with
this invention. See, e.g., N. C. Cohen et al, "Molecular Modeling Software and Methods for
Medicinal Chemistry", J. Med. Chem., 33:883-894 (1990). See also, M. A. Navia and M. A.
Murcko, "The Use of Structural Information in Drug Design", Current Opinions in
Structural Biology, 2:202-210 (1992). For example, where the structures of test compounds
are known, a model of the test compound may be superimposed over the model of the
structure of the invention. Numerous methods and techniques are known in the art for
performing this step, any of which may be used. See, e.g., P.S. Farmer, Drug Design,
Ariens, E.J., ed., Vol. 10, pp 119-143 (Academic Press, New York, 1980); U.S. Patent No.
5,331,573; U.S. Patent No. 5,500,807; C. Verlinde, Structure, 2:577-587 (1994); and I. D.
Kuntz, Science, 257:1078-1082 (1992). The model building techniques and computer
evaluation systems described herein are not a limitation on the present invention.

Thus, using these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided.

Moreover, the need for actual synthesis of many compounds is effectively eliminated.

In another aspect, the undecaprenyl pyrophosphate synthase structure of the invention permit the design and identification of synthetic compounds and/or other

molecules which are characterized by the conformation of the undecaprenyl pyrophosphate synthase of the invention. Using known computer systems, the coordinates of the undecaprenyl pyrophosphate synthase structure of the invention may be provided in machine readable form, the test compounds designed and/or screened and their conformations superimposed on the structure of the undecaprenyl pyrophosphate synthase of the invention. Subsequently, suitable candidates identified as above may be screened for the desired undecaprenyl pyrophosphate synthase inhibitory bio-activity, stability, and the like.

Once identified and screened for biological activity, these inhibitors may be used therapeutically or prophylactically to block undecaprenyl pyrophosphate synthase activity, and thus, overcome bacterial resistance to antibiotics, for example, of the beta-lactam class, eg. imipenem, penicillins, cephalosporins, etc. by using an entirely different mechanism of attacking bacteria in diseases produced by bacterial infection.

15 Abbreviations used herin

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13	Abbreviations used nerm		
	ATP	adenosine triphosphate	
	ADP	adenosine diphosphate	
	AR	androgen receptor	
	CAT	chloramphenicol acyltransferase	
20	CBP	CREB binding protein	
٠.	cDNA	complementary DNA	
	DBD	DNA binding domain	
	DMSO	dimethyl sulfoxide	
	DNA	deoxyribonucleic acid	
25	DTT	dithiothreitol	
	EDTA	ethylenediaminetetraacetic acid	
	ER	estrogen receptor	
	FPP	farnesyl pyrophosphate	
	GST	glutathione S-transferase	
30	HEPES	N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid	
	HSP	heat shock protein	
	IPP	Isopentenyl pyrophosphate	
	kDa	kilodalton(s)	
	LBD	ligand binding domain	
35	MR	mineralcorticoid receptor	

	NDP	nucleotide diphosphate
	NID	nuclear receptor interaction domain
	NTP	nucleotide triphosphate
	PAGE	polyacrylamide gel electrophoresis
5	PCR	polymerase chain reaction
	pI	isoelectric point
	PPAR · · ·	peroxisome proliferator-activated receptor
	PR .	progesterone receptor
	RAR	retinoid acid receptor
10	RXR	retinoid X receptor
	SDS	sodium dodecyl sulfate
	SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis
	TIF2	transcription intermediary factor 2
	TR	thyroid receptor
15	UPPS	undecaprenyl pyrophosphate synthase
	VDR	vitamin D receptor

Amino Acid Abbreviations used herein

	Single-Letter Code	Three-Letter Code	<u>Name</u>
20	Α	Ala	Alanine
	V	Val	Valine
	L	Leu	Leucine
	I	Ile .	Isoleucine
	. P	Pro	Proline
25	F	Phe	Phenylalanine
	· W	Trp	Tryptophan
	M	Met	Methionine
	G	Gly	Glycine
	S	Ser	Serine
30	T	Thr	Threonine
	С	Cys	Cysteine
	Y	Tyr	Tyrosine
	N	Asn	Asparagine
	Q	Gln	Glutamine
35	D	Asp	Aspartic Acid

WO 03/048733		PCT/US02/38715	
E	Glu	Glutamic Acid	

~		O.G	0.4
K		Lys	Lysine
R		Arg	Arginine
H.	·	Hic	Histidine

Functionally Equivalent Codons

	Amino Acid			Codons
	Alanine	Ala	Α	GCA GCC GCG GCU
5	Cysteine	Cys	·C	UGC UGU
	Aspartic Acid	Asp	D	GAC GAU
	Glumatic acid	Glu	E	GAA GAG
	Phenylalanine	Phe	F	ບບບບບບ
	Glycine	Gly	G	GGA GGC GGG GGU
	Histidine	His	, H	CAC CAU
10	Isoleucine	Ile	I	AUA AUC AUU
	Lysine	Lys	. K	AAA AAG
	Methionine	Met	M	AUG
	Asparagine	Asn	N	AAC AAU
15	Proline	Pro	P	CCA CCC CCG CCU
	Glutamine	Gln	Q	CAA CAG
	Threonine	Thr	T	ACA ACC ACG ACU
	Valine	Val	V	GUA GUC GUG GUU
	Tryptophan	Trp	W	UGG
	Tyrosine	Tyr	Y	UAC UAU
	Leucine	Leu	L	UUA UUG CUA CUC CUG CUU
20	Arginine	Arg	R	AGA AGG CGA CGC CGG CGU
	Serine	Ser	S	ACG AGU UCA UCC UCG UCU

The following examples illustrate various aspects of this invention. These examples

do not limit the scope of this invention that is defined by the appended claims.

Example 1- <u>Expression and purification of UPPS prenyltransferase from Streptococcus</u> <u>pneumoniae in Escherichia coli</u>

UPPS from Streptococcus pneumoniae with an additional 20 residues at the amino terminus that include the hexa-histidine tag was over expressed in E. coli, strain BL21(DE3), and purified by NiNTA (nickel nitrilo-tri-acetic acid) column. A plasmid pET28-UPPS was transformed into E. coli BL21 (DE3). For expression E. coli BL21 (pET28-UPPS) was grown at 37 °C in LB medium containing 1% glucose and 50 ug/ml kanamycin to OD600 0.5 and then induced with 1 mM IPTG for 3 hrs. The induced cultures

were harvested by centrifugation. The cell paste was suspended in 25 ml Buffer A (10mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5) containing 0.1mg/ml of lysozyme. After incubating on ice 30 min, the cell suspension was put through 4 cycles of sonication, freeze and thaw. The lysate was centrifuged and the supernatant applied to the NiNTA column. The column was washed with 18 ml of Buffer A and 12.5ml of Buffer B (100 mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5). The His-tagged UPPS was eluted with 10 ml of Buffer C (500 mM imidazole, 50mM Na-phosphate, 0.5M NaCl pH7.5). The eluted His-UPPS was dialyzed overnight at 4 °C against 2L of 50mM Tris-HCl pH 7.5, 0.2M NaCl and 1mM EDTA. The soluble polypeptide includes 272 amino acid residues with a molecular weight of 29,000. This product was greater than 95% pure by SDS PAGE, has the desired enzymatic activity, and N-terminal amino acid analysis confirmed its identity.

1.A. Measurement of UPPS activity

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Enzymatic activity of UPPS was assayed by measuring the incorporation of (1-14C)IPP (isopentenyl diphosphate) into butanol-soluble materials from the condensations of FPP and (1-14C)IPP using a butanol extraction assay (Shimizu et al. 1998). A typical assay of 100 ul contained 100 mM Tris-HCl, pH7.5, 50 mM KCl, 0.5 mM MgCl2, 0.05% Triton X-100, 0.5 uM FPP, 3.6 uM (1-14C)IPP, and 6 nM purified S. pneumoniae His-UPPS. The reaction was incubated at 25 °C for 25 min and stopped by addition of EDTA to 50 mM. The reaction was extracted with equal volume of 1-butanol and the radioactivity in the butanol phase was measured with a liquid scintillation counter (Shimizu, N., T. Koyama, and K. Ogura. (1998) J Biol. Chem. 273:19476-19481).

25 1.B. Ligand binding to UPPS

It is also possible to define ligand interactions with UPPS in experiments that are not dependent upon enzyme catalyzed turnover of substrates. This type of experiment can be done in a number of ways:

30 <u>1.B.1. Effects of ligand binding upon enzyme intrinsic fluorescence</u> (e.g. of tryptophan)
Binding of either natural ligands or inhibitors may result in enzyme conformational changes which alter enzyme fluorescence. Using stopped-flow fluorescence equipment, this can be used to define the microscopic rate constants that describe binding. Alternatively, steady-state fluorescence titration methods can yield the overall dissociation constant for binding in the same way that these are accessed through enzyme inhibition experiments.

Example 2 <u>Crystallization</u>, structure determination and refinement of a crystal structure of <u>UPPS from Streptococcus pneumoniae</u>

2.A. Crystallization '

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Single crystals of native UPPS grew from sitting or hanging drops prepared by mixing 2 µL protein (9.5 mg/ml in 50mM Tris-HCl, pH 7.5, 0.2M NaCl, 1mM EDTA) with 2µL of reservoir solution containing either 10-20% ethanol, 0.1M Tris-HCl, pH 8.5 or 4-5% PEG6000, 0.1M HEPES, pH 7.5. The drops were left to equilibrate at room temperature against 500µL of the reservoir solution. The crystals belong to the orthorhombic crystalline form having a space group P2₁2₁2₁ with unit cell parameters: a = 59.6Å, b = 118.0Å, c = 178.2Å, and two 60 kDa dimers in the asymmetric unit. Some crystals were found to belong to the orthorhombic crystalline form having a space group I2₁2₁2₁ with the similar cell parameters as the primitive cell. In the primitive cell, a pseudo-translation of nearly 1/2, 1/2, 1/2 along the cell edges, results in a diffraction pattern in which the h + k + l = odd are, on the average, markedly weaker than the h + k + l = even reflections resulting in a pseudo body centered lattice. The crystals were quickly transferred to a solution of mother liquor containing 30% xylitol as cryo-protective agent and flash frozen under the cold stream before data collection. The Se-Met substituted protein was expressed in E. coli fed with an amino acid mixture that inhibited the endogenous biosynthesis of methionine and forced the uptake of selenium-labeled methionine from the medium. The protein was crystallized under similar conditions with the exception that the crystallization drops were flushed with argon gas before sealing them in order to prevent oxidation. The crystal structure of UPPS in complex with IPP was determined using native crystals soaked at room temperature for 20-30 minutes in mother liquor containing 2-3mM IPP and 2mM MgCl₂. The co-crystals of UPPS in complex with the substrate IPP crystals belong to the orthorhombic crystalline form having the space groups P2₁2₁2₁ and I2₁2₁2₁, similar to the native crystal. The cocrystals of UPPS in complex with the substrate FPP were grown at room temperature from sitting drops prepared by mixing 2uL of protein solution (~10mg/ml, 2mM FPP, 1,mM MgCl2, 50mM Tris-HCl pH 7.5 and 200mM NaCl) with 2uL of reservoir solution containing 100mM sodium cacodylate, pH 6.4, 120-240 mM sodium acetate. These crystals belong to the monoclinic crystalline form having a space group P21 with unit cell dimensions a = 58.1 Å, b = 44.6 Å, c = 115.5 Å, $\beta = 98.7^{\circ}$.

2.B. X-ray diffraction data collection

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A native UPPS crystal structure was determined by multiwavelength anomalous diffraction, MAD, using the K absorption edge of selenium incorporated into the amino acid methionine. Three diffraction data sets to 2.3Å resolution were collected at the NSLS's X12C beamline. The wavelengths were determined by analyzing the x-ray fluorescence of the UPPS crystal around the selenium absorption edge. These correspond to the peak (0.9795Å), the inflection point (0.9791Å) and at a remote wavelength on the high-energy side of the edge (0.9500Å). Diffraction intensities from each wavelength were independently integrated, merged and scaled using DENZO/SCALEPACK (Otwinowsky, et al. (1999) *Methods in Enzymology* Vol. 267). Diffraction data from UPPS in complex with FPP or IPP were collected at the 17ID beamline at the Advanced Photon Source, APS, at Argonne National Laboratory, using 1.000Å wavelength.

2.C. Structure Determination

A selenium substructure was determined by automatic Patterson map peak search and peak correlation implemented in the program SOLVE (Terwilliger, T. C., and Berendsen, J. (1999) Acta Crystallogr. D55: 849-861). A Fourier map was calculated to 2.7Å resolution using phases calculated from 15 of the possible 24 Se sites in the asymmetric unit. After solvent modification, this map afforder the determination of the boundaries of the four monomers and tracing of the polypeptide chains. The tracing was used to find the rotation and translation transformations used in 4-fold electron density averaging (CCP4, DM). The improved, averaged map was also used in tracing of the chains.

2.D. Model Building and Refinement

This averaged electron density map was of high quality and afforded the complete tracing of the four molecules using the interactive computer graphics program O (Jones, T.A. et al. (1991) Acta Crystallogr. A47: 110-119). The initial model was refined against diffraction data collected at the remote wavelength by successive rounds of simulated annealing with torsion angle dynamics, positional refinement and restrained B-factor refinement using CNS (A. Brunger et al., Science, 235: 458-460 (1987)) followed by manual intervention. The refinement and manual rebuilding was monitored by the quality of the 2Fo-Fc and Fo-Fc electron density maps and the value of the crystallographic R and R_{free}. At the beginning of the refinement, the four molecules in the asymmetric unit (A, B C, and D) were forced to obey strict non-crystallographic symmetry. This constraint was released as the refinement proceeded.

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A final R is 0.20 and the R_{free} is 0.25 for 53,642 reflections to 2.3Å resolution. The rms deviation from the reference bond lengths and bond angles (Engh & Huber (1991) Acta Crystallogr. A47: 392-400) are 0.01 and 1.4, respectively. The refined model includes residues 17-72, 77-248 in molecule A, 17-72, 79-246 in molecule B, 17-73, 77-248 in molecule C and 18-73, 78-246 in molecule D according to the amino acid sequence SEQ ID NO:1. The N-terminal residues 1-16 were disordered in the four molecules. Also were disordered the residues in the vicinity of the loop formed by amino acids 72-80. A number of conserved amino acids that may form part of the active site (see below) are located in this region. The six residues 247-252 at the C-terminus were also disordered. In the refined model, all the main chain conformations fall in the "allowed" regions of the Ramachandran plot. Molecules A and B form one of the dimers and molecules C and D the second dimer in the asymmetric unit. The Ca-carbon atoms of the two pairs of molecules in each dimer, molecules A and B, and C and D, superimpose with a rms deviation of 1.2Å and 1.1Å, respectively, with very large differences at the N- (6.1Å) and C-termini (1.5Å), the turn formed by residues 35-41 (1.2Å), the long helix formed by residues 79-104 (7.1Å), the short turn formed by residues 115-127 (2.2Å), and residues 157-171 (1.7Å) that form an α -helix and a turn. Omitting these residues from the comparison gives a rms of 0.3Å or both pairs of molecules. The turn formed by residues 35-41 (1.2Å) in molecule A has no crystal contacts or contacts with the partner in the dimer, however, in molecule B it is making contacts with the sane region in molecule D. The long helix from 79-104 is not making contacts in molecules A or D but in C is contacting residues in the region of B177, and in B is contacting D117 of a symmetry related molecule; this region leads to a disordered loop that may be involved in substrate binding. B115 region is in contact with symmetry related D119-D121, and D115 is contacting symmetry related B85-B88 region. A166 is in contact with symmetry related B240, C166 is in contact with symmetry related D240, but neither B166 nor D166 are making any crystal contacts.

A crystal structure of a UPPS in complex with FPP was determined by molecular replacement with the program package AMoRe (Navaza, J. (1994) Acta Cryst. A50, 157-163) using the native structure as search model and refined as described before. The cross rotation and translation searches were carried using data from 20Å to 4Å resolution and a radius of integration of 20Å. The top two solutions of the cross rotation function corresponding to the tow molecules in the dimer in the asymmetric unit were unambiguously discriminated from the noise peaks. The search for the correct translation for each molecule in the asymmetric unit produced a solution for the tetramer with an R-factor

of 0.60 and a correlation coefficient of 0.34 after rigid body refinement in. The crystal structure of the complex with IPP was determined by Fourier methods.

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All documents cited herein and patent applications to which priority is claimed are incorporated by reference herein in their entirety. This invention is not to be limited in scope by the specific embodiments described herein. Indeed, various modifications of the invention in addition to those described herein will become apparent to those skilled in the art from the foregoing description. Such modifications are intended to fall within the scope of the appended claims. The disclosures of the patents, patent applications and publications cited herein are incorporated by reference in their entireties.

SEQUENCE LISTING

```
(1) GENERAL INFORMATION:
             (i) APPLICANT: Néstor O. Concha, and Cheryl A. Janson
   5
             (ii) TITLE OF INVENTION: Novel UPPS Enzyme
             (iii) NUMBER OF SEQUENCES: 1
             (iv) CORRESPONDENCE ADDRESS:
                   (A) ADDRESSEE: GlaxoSmithKline Corporation
                         (B) STREET: 709 Swedeland Road - P.O. Box 1539
  10
                         (C) CITY: King of Prussia
                         (D) STATE: Pennsylvania
                         (E) COUNTRY: USA
                         (F) ZIP: 19406-2799
15
            (v) COMPUTER READABLE FORM:
                   (A) MEDIUM TYPE: Floppy disk
                   (B) COMPUTER: IBM PC compatible
                   (C) OPERATING SYSTEM:
  20
                   (D) SOFTWARE:
           (vi) CURRENT APPLICATION DATA:
                   (A) APPLICATION NUMBER:
                   (B) FILING DATE:
  25
                   (C) CLASSIFICATION:
          (vii) PRIOR APPLICATION DATA:
                   (A) APPLICATION NUMBER:
                   (B) FILING DATE:
  30
                   (A) APPLICATION NUMBER:
                   (B) FILING DATE:
         (viii) ATTORNEY/AGENT INFORMATION:
  35
                   (A) NAME:
                   (B) REGISTRATION NUMBER:
```

(C) REFERENCE/DOCKET NUMBER:

35.

231

	(ix) TE	LECOMMUNICA	rion inform	ATION:	
		(A) TELEPHO	ONE:		
	•	(B) TELEFA	X:	6 9	
5	126		•		
	(2) INFORMA	TION FOR SE	Q ID NO:1:		
	(i) S	EQUENCE CHA	RACTERISTIC	S:	
10		•	LENGTH: 272		s
		(B)	TYPE: amino	acid	
		(C)	STRANDEDNES	s:	
		(D).	TOPOLOGY: 1	inear	
			1	•	
15	(ii)	MOLECULE TY	PE: protein		•
				· · · · · · · · · · · · · · · · · · ·	
	(iii)	SEQUENCE I	DESCRIPTION:	SEQ ID NO:	
20	-20	-10	1	11	21
	MGSSHHHHHH	SSGLVPRGSH	MFGFFKKDKĄ	VEVEVPTQVP.	AHIGIIMDGA
	31	41	51	61	71
			ALQTVTKAAN	KLGVKVITVY	AFSTENWTRE
25			•		
	81	91	101	111	121
	DQEVKFIMNL	PVEEADNAAL	ELHANNVKIQ	MIGETDRLPK	QTFEALTKAL
	131	141	151	161	171
30			AEITQALKLI		
				•	
	181	191	201	211	
	NYLFTQHLPK	DLRDPDLIIR	TSGELRLSNF	LPWQGAYSEL	YFTDTLWPD

251

241 DEAALQEAIL AYNRRHRRFG GV

Figure 1A

Figure 1B

Figure 2A

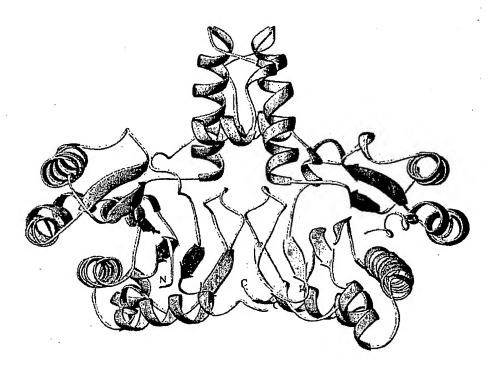


Figure 2B

UPS (S. pneumoniae)

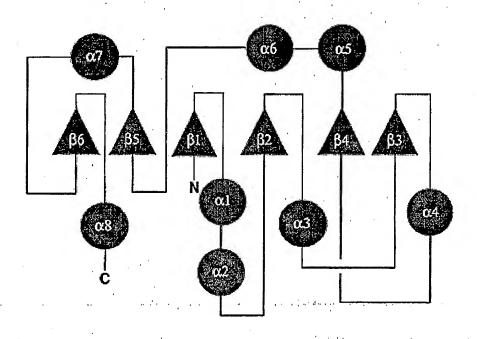
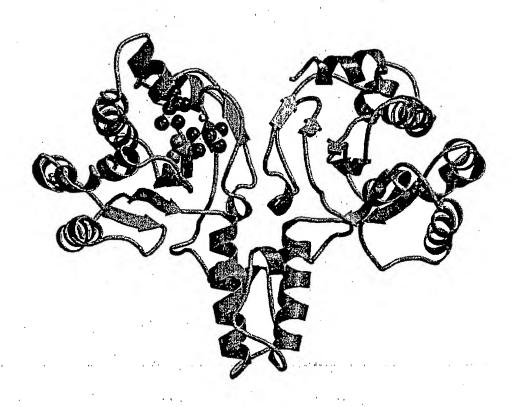


Figure 3A



PCT/US02/38715

Figure 3B

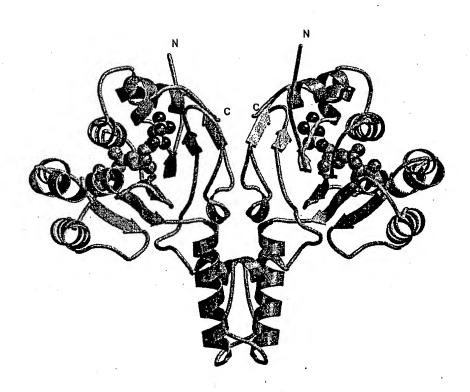


Figure 4A



Figure 4B

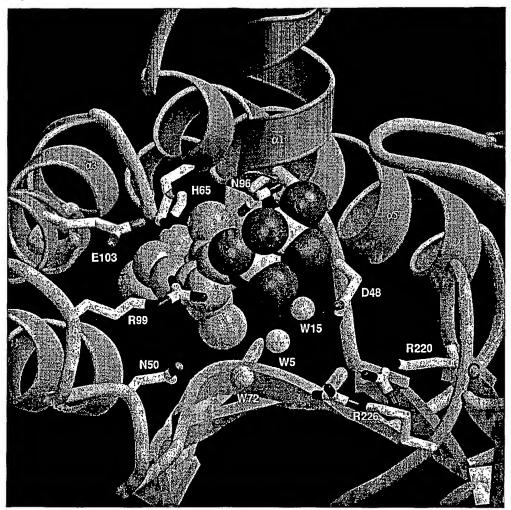


Figure 5

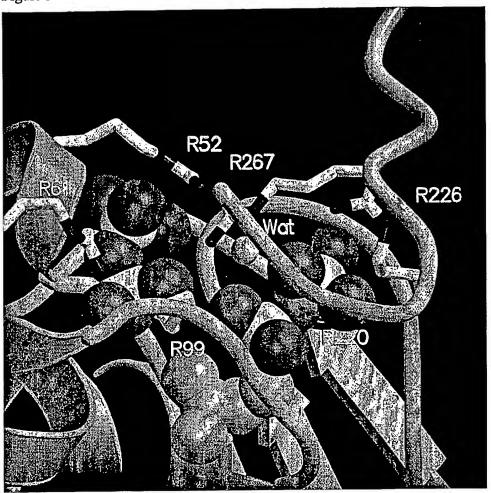


TABLE I

Table IA. Atomic coordinates of native UPPS structure

5 Table IB. Atomic coordinates of active of UPPS in complex with FPP Table IC. Atomic coordinates of active of UPPS in complex with IPP

TABLE II

Table IIA. Interatomic distances in an active site of the native UPPS

Table IIB. Interatomic distances in an active site of UPPS in complex with FPP Table IIC. Interatomic distances in an active site of UPPS in complex with IPP

TABLE III

Table IIIA. Interatomic angles in an active site of the native UPPS

Table IIIB. Interatomic angles in an active of UPPS in complex with FPP Table IIIC. Interatomic angles in an active of UPPS in complex with IPP

Legend:

- Under the heading ATOM appears a "atom number" (e.g. 1,2,3,4...etc) and the "atom name" (e.g. CA, CB, N,... etc) such that to each "atom name" in the coordinate list corresponds an "atom number".
- Under the heading RESIDUE appears a three-letter "residue name" (e.g. THR, ASP, etc), a "chain identifier" represented by a capital letter (e.g. A, B, C D, etc) and a "residue number", such that to each residue (or amino acid) in the amino acid sequence of the particular protein in the structure corresponds a name that identifies it, a number according to its position along the amino acid sequence, and a chain name. The chain name identifies a particular molecule in the crystal structure. For instance, if there are more than one molecule that form the unit that is repeated throughout the crystal lattice, then each unit is identified
 as molecule A, or molecule B, or molecule C, etc.
 - 3. Under the headings X, Y, or Z appear the Cartesian coordinates of the atoms in the structure.

4. Under the heading OCC appears the "occupancy factor" for each atom. If the entity is present and observed in the structure then occupancy of 1.00 is assigned to it. If the atom is present but not observed, occupancy of 0.00 is assigned to it. Also, factors between 0.00 and 1.00 are also acceptable and represent the degree of confidence in observing that atom a that particular position.

5. Under the heading B appears the "B-factor" or "temperature factor" which can adopt, in principle, any value. It is meant to represent the atomic displacement around that position.

10 Table IA

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Atomic coordinates of native UPPS 118.000 90.00 90.00 90.00 178.200 CRYST1 59.600 OCC B X <u>z</u> MOTA RESIDUE · <u>X</u> 1.00 93.58 87.195 103.592 18.414 THR A 17 CB · 1 18.502 87.203 105.024 1.00 94.14 15 OG1 THR A 17 2 1.00 93.23 88.014 103.149 17 17.190 CG2 THR A 3 1.00 89.94 84.999 103.347 19.637 17 С THR A 4 1.00 91.11 85.538 104.017 20.525 17 0 THR A 5 1.00 90.66 85.002 103.724 17 17.169 6 N THR A 85.723 103.077 1.00 91.60 20. THR A 17 18.311 7 CA 83.783 102.808 1.00 86.41 19.761 GLN A 18 N 8 1.00 80.31 20,949 82.945 102,991 GLN A 18 CA 1.00 83.93 83.757 102.767 22.219 CB $\mathtt{GLN} \cdot A$ 18 10 84.548 101.482 1.00 89.19 22.233 11 CG GLN A 18 1.00 94.65 85.747 101.583 23.150 25 18 12 CD GLN A 1.00 95.46 24.334 85.612 101.914 OE1 GLN A 18 13 86.934 101.306 1.00 95.13 22.608 NE2 GLN A 18 14 1.00 73.54 82.433 104.429 20.918 15 С GLN A 18 81.846 104.922 1.00 71.59 18 21.875 GLN A 0 16 1.00 64.52 82.678 105.085 19.793 30 N VAL A 19 17 1.00 56.20 82.272 106.464 19.567 VAL A 19 18 CA 1.00 53.44 83.445 107.244 18.912 VAL A 19 19 CB 82.935 108.392 1.00 51.55 18.089 CG1 VAL A 19 20 84.383 107.750 1.00 55.06 19.991 CG2 VAL A 19 21 81.024 106.548 1.00 50.21 19 18.667 35 С VAL A 22 1.00 47.54 80.997 105.979 17.570 23 0 VAL A 19 79.967 107.243 1.00 42.84 19.132 24 N PRO A 20 79.772 107.880 1.00 36.61 20.450 CD PRO A 20 25 78.763 107.358 1.00 35.73 18.304 20 26 CA PRO A

19.193

PRO A

40

27

CB

20

77.808 108.161

1.00 36.35

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                                                        1.00 30.89
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          CG1 ILE A
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          CG
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                ARG A
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                ARG A
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      111
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           NE
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            NH1 ARG A
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35.173 70.594 126.743 1.00 72.13
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          CE2 TRP A
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          CE3 TRP A
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                               28.774
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	158	CD	ARG	A	37	33.261		134.440		66.92
	159	NE	ARG	A	37	32.981		133.044		70.08
	160	CZ	ARG	A·	37	33.178		132.027		74.26
5	161	NH1	ARG	A	37	33.649	79.893	132.247	1.00	73.92
	162	NH2	ARG	A	37	32.926	81.506	130.783	1.00	75.48
	163	С	ARG	A	37	34.096	79.111	138.220	1.00	60.36
	164	0	ARG	A	37	33.850	80.006	139.026	1.00	63.86
	165	N	MET	Α	38	34.345	77.863	138.599	1.00	62.29
10	166	CA	MET	A	38	34.369	77.489	140.011	1.00	64.24
	167	СВ	MET	A	38	35.506	78.227	140.724	1.00	67.10
	168	CG	MET	A	38	36.885	77.800	140.280	0.50	70.38
	169	SD	MET	A	38	37.169	76.085	140.705	0.50	77.34
	170	CE	MET	A	38	38.285	76.262	142.112	0.50	76.14
15	171	С	MET	Α	38	33.050	77.799	140.716	1.00	63.85
	172	0	MET	A	38	33.003	77.880	141.939	1.00	65.90
•	173	N	GLN	A	39	31.985	77.974	139.944	1.00	63.31
	174	CA	GLN	A	39	30.671	78.290	140.492	1.00	62.45
	175	СВ	GLN	A	39	30.023	79.381	139.648	1.00	61.29
20	176	CG	GLN		39	30.575	80.745	139.923	1.00	69.13
	177	CD	GLN		39	30.115	81.260	141.266	1.00	76.78
	178	OE1	GLN	A	39	28.943	81.601	141.444	1.00	81.67
	179	NE2	GLN	A	39	31.026	81.303	142.228	1.00	80,44.
	180	С	GLN		39	29.767	77.063	140.536	1.00	62.86
25	181	0	GLN	A	39	30.064	76.051	139.915	1.00	63.48
	182	N	PRO		40	28.649	77.133	141.279	1.00	64.92
	183	CD	PRO	A	40	28.105	78.262	142.059	1.00	65.41
	184	CA	PRO	A	40	27.753	75.972	141.343	1.00	65.47
	185	СВ	PRO	A	40	26.764	76.367	142.442	1.00	62.80
30	186	CG	PRO		40	26.657	77.854	142.265	1.00	64.53
		С	PRO	A	40	27.072	75.728	139.987	1.00	65.74
	188	0	PRO	A	40	26.856	76.675	139.219	1.00	64.28
	189	N	ARG	A	41	26.747	74.467	139.694	1.00	64.20
	190	CA	ARG	Α.	41	26.098	74.111	138.434	1.00	66.35
35	191	СВ	ARG		41	25.553	72.678	138.478	1.00	69.33
	192	CG	ARG		41	26.592	71.590	138.246	1.00	78.61
	193	CD	ARG	A	41	25.997	70.436	137.431	1.00	86.11
	194	NE	ARG		41	25.524		136.120	1.00	92.86
	195	CZ	ARG		41	24.937		135.204	1.00	95.17
40	196		ARG		41	24.737		135.439		98.23
. •	197		ARG		41	24.542		134.048	1.00	93.83
	198	С	ARG		41			138.088	1.00	65.18
		0			41	24.770	75.425	136.927	1.00	65.36

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75.441 139.101
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              VAL A 42
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	249	0	GLY	A	48	20.954	79.94	3 127.950	1.00 42.20
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	254	SD	MET	A	49	16.447	80.362	132.865	0.50 50.86
	255	CE	MET	A	49	17.404	80.914	134.277	0.50 47.30
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5	505	СВ	LYS		85	16.847	69.087	139.502	0.50 58.82
•	506	CG	LYS		85	16.254	69.391	140.860	0.50 63.20
	507	CD	LYS		85	15.406	68.227	141.337	0.50 64.80
	508	CE	LYS		85	15.390	68.153	142.852	0.50 66.73
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	1368	CB	ARG	A	193		7.484	70,458	110.010	1.00	32.16
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	2003	NH2	ARC	3 В	37	43.836	56.507	93.925	1.00	39.69
	2004	С	ARC	3 B	37	41.556	60.571	87.386	1.00	34.97
	2005	0	ARG	; в	37	42.055	59.811	86.561	1.00	28.07
5	2006	N	MET	В	.38	40.712	61.548	87.057	1.00	35.33
	2007	CA	MET	В	38.	40.308	61.818	85.681	1.00	37.27
	2008	СВ	MEI	В	38	41.471	62.395	84.874	1.00	38.26
	2009	CG	MET	В	38	41.874	63.792	85.305	1.00	43.26
	2010	SD	MEI	. B	38 -	43.320	64.442	84.413	1.00	50.85
10	2011	CE	MET	В	38	42.639	64.685	82.741	1.00	42.32
	2012	С	MET	' B	38	39.774	60.581	84.983	1.00	41.75
	2013	0	MEI	' В	38	40.097	60.322	83.828	1.00	44.59
	2014	N	GLN	В	39	38.968	59.808	85.694	1.00	38.24
	2015	CA	GLN	В	39	38.368	58.614	85.128	1.00	39.36
15	2016	CB	GLN	В	39.	38.766	57.364	85.937	1.00	40.98
	2017	CG	GLN	ľΒ	39	40.240	56.980	85.829	1.00	43.52
	2018	CD	GLN	В	39	40.588	55.705	86,589	0.50	43.10
	2019	OE1	GLN	В	39	40.396	55.611	87.803	0.50	39.90
	2020	NE2	GLN	В	39	41.112	54.718	85.870	0.50	44.08
20	2021	С	GLN	В	39	36.858	58.812	85.203	1.00	40.23
	2022	0	GLN	В	39	36.375	59.639	85.969	1.00	34.98
	2023	N	PRO	В	40	36.092	58.072	84.391	1.00	42.21
	2024	CD	PRO	В	40	36.495	57.164	83.304	1.00	48.07
	2025	·CA	PRO	В	40	34.637	58.230	84.443	1.00	45.23
25	2026	CB	PRO	В	40	34.154	.57.388	83.258	1.00	47.19
	2027	CG	PRO	В	40	35.238	56.369	83.076	1.00	50.59
	2028	С	PRO	В	40	34.067	57.766	85.798	1.00	44.28
	2029	0	PRO	В	40	34.635	56.881	86.441	1.00	38.91
	2030	N	ARG		41	32.959	58.376	86.222	1.00	44.37
30	2031	CA	ARG	В	41	32.319	58.058	87.504	1.00	49.09
	2032	CB	ARG			30.968	58.7 7 7	87.608	1.00	51.36
	2033	CG	ARG		41	30.302	58.631	88.975	1.00	63.60
	2034	CD	ARG		41	29.289	59.748		1.00	66.85
25	2035	NE	ARG		41	28.693	59.591	90.588	1.00	67.64
35	2036	CZ	ARG		41	28.506	60.590	91.445	1.00	71.31
	2037		ARG		41	28.869	61.826	91.117		71.73
	2038		ARG		41	27.973	60.351			72.69
	2039	С	ARG		41	32.137	56.563		1.00	44.94
40	2040	0	ARG		41		56.114			44.70
40	2041	N ~-	VAL		42	31.946	55.799			45.95
	2042	CA	VAL		42	31.782	54.356			48.03
	2043	СВ	VAL		42	31.646	53.729			52.94
	2044	CG1	VAL	В	42	31.015	52.363	85.518	1.00	55.31

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	2091	N	MET	В	49	33.744	49.559	95.554	1.00	24.06
5	2092	CA	MET	В	49	33.517	48.144	95.869	1.00	28.88
	2093	СВ	MET	В	49	33.130	47.331	94.621	1.00	31.04
	2094	CG	MET	В	49.	31.635	47.133	94.381	1.00	39.52
	2095	SD	MET	В	49	31.234	45.702	93.276	0.50	35.36
	2096	CE	MET	В	49	31.697	46.395	91.762	1.00	37.74
10	2097	С	MET	В	49	34.793	47.551	96.477	1.00	30.80
•	2098	0	MET	В	49	34.734	46.752	97.413	1.00	35.99
	2099	N	GLU	В	50	35.950	47.940	95.952	1.00	33.55
	2100	CA	GLU	В	50	37.221	47.426	96.480	1.00	31.25
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15	2102	CG	GLU	В	50	38.554	47.294	94.256	1.00	38.13
	2103	CD	GLU	В	50	38.789	45.789	94.313	1.00	47.32
	2104	OE1	GLU	В	50	39.537	45.337	95.217	1.00	47.00
	2105	OE2	GLU	В	50	38.232	45.061	93.456	1.00	42.37
	2106	С	GLU	В	50	37.384	47.898	97.905	1.00	30.84
20	2107	0	GLU	В	50	37.708	47.110	98.796	1.00	31.48
	2108	N	ALA	В	51	37.156	49.193	98.120	1.00	30.50
	2109	CA	ALA	В	51	37.286	49.768	99.453	1.00	32.09
	2110	CB	ALA	В	51	36.911	51.262	99.426	1.00	32.81
	2111	С	ALA	В	51	36.395	49.008	100.436	1.00	27.96
25	2112	0	ALA	В	51	36.814	48.700	101.548	1.00	30.77
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	2114	CA	LEU	В	52	34.257	47.957	100.891	1.00	25.95
	2115	СВ	LEU	В	52	32.848	47.823	100.274	1.00	26.02
	2116	CG	LEU	В	52	31.809	47.122	101.177	1.00	26.29
30	2117	CD1	LEU	B	- 52	31.723	47.839	102.524	1.00	18.74
	2118	CD2	LEU	В	52	30.432	47.111	100.508	1.00	24.68
	2119	С	LEU	В	52	34.831	46.581	101.182	1.00	27.37
	2120	0	LEU	В	52	34.856	46.154	102.332	1.00	23.49
	2121	N	GLN	В	53	35.307	45.892	100.150	1.00	26.27
35	2122	CA	GLN	В	53	35.886	44.574	100.374	1.00	32.31
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	2124	CG	GLN	В	53	36.905	42.525	99.236	1.00	39.18
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	2126	OE1	GLN	В	53	34.594	41.928	99.057	1.00	37.18
40	2127	NE2	GLN	В	53	36.105	40.319	98.580	1.00	38.63
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5	2257	CA	ALA	В	71		25.388	53.675	98.954	1.00 50.72
	2258	CB	ALA	В	71		24.844	52.879	97.783	1.00 51.20
	2259	С	ALA	В	71	•	25.098	55.181	98.738	1.00 58.46
,	2260	0	ALĀ	В	71		23.988	55.541	98.331	1.00 58.45
	2261	N	PHE	В	72		26.101	56.028	99.017	1.00 63.98
10	2262	CA	PHE	В	72		25.996	57.485	98.850	1.00 64.38
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	2265	CD1	PHE	В	72		27.615	60.047	97.313	0.00 60.50
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15	2267	CE1	PHE	В	72		27.673	61.421	97.061	0.00 59.87
	2268	CE2	PHE	В	72		25.346	61.416	96.509	0.00 59.87
	2269	CZ	PHE	В	72		26.536	62.101	96,661	0.00 59.69
	2270	C =	PHE	В	72		24.589	57.985	99.163	1.00 67.12
	2271	0	PHE	В	72		24.386	58.852	100.010	1.00 71.18
20	2272	N	ARG	В	79		21.453	60.062	86.391	1.00 98.48
	2273	CA	ARG	В	79		21.443	59.714	84.973	1.00 99.65
	2274	CB	ARG	В	79		22.698	60.270	84.293	1.00 99.37
	2275	CG	ARG	В	79		23.990	60.014	85.046	1.00100.00
	2276	. CD	ARG	В	79	٠.	25.186	60.551	84.273	1.00100.00
25	2277	NE	ARG	В	79		25.372	59.857	83.000	1.00100.00
	2278	CZ	ARG	В	79		26.289	60.183	82.091	1.00100.00
	2279	NH1	ARG	В	79		27.115	61.203	82.307	1.00100.00
	2280	NH2	ARG	В	79		26.382	59.486	80.962	1.00100.00
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30	2282	0	ARG	В	79		22.125	57.418	85.254	1.00 99.98
	2283	N	PRO	В	80		20.342	57.775	83.918	1.00100.00
	2284	CD	PRO	В	80		19.376	58.690	83.280	1.00100.00
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35	2287	CG	PRO	В	80		18.260	57.748	82.867	1.00100.00
	2288	С	PRO	В	80		21.185	55.466	83.141	1.00 99.89
	2289	0	PRO		80		21.150	54.272	83.442	1.00 98.69
	2290	N	ASP	В	81		22.192	55.998	82.453	1.00100.00
.0		. CA	ASP	В	81		23.305	55.159	82.024	1.00100.00
40	2292	CB	ASP	В	81		24.022	55,775	80.822	1.00100.00
	2293	CG	ASP		81		24.599	54.720	79.890	1.00100.00
	2294		ASP		81		23.795	53.965	79.291	1.00 99.35
	2295	OD2	ASP	В	81		25.844	54.638	79.768	1.00 98.37

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		2296	C	AS	P E	81		24.292	54.917	83.162	1.00 99.36
		2297	0	AS	P E	81		25.319	54.260	82.990	1.00 99.22
		2298	N	GL	N B	82		23.969	55.458	84.328	1.00 98.43
		2299	CA	GL	ŃВ	82		24.800	55.284	85.505	1.00 98.86
	5	2300	CB	GL	ΝĖ	82		25.355	56.630	85.979	1.00 98.97
		2301	CG	GL	N B	82		26.328	56.526	87.151	1.00 98.76
		2302	CD	GL	N B	82		26.671	57.879	87.755	1.00 98.93
		2303	OE	1 GL	N _. B	82		27.055	58.809	87.041	1.00 98.73
		2304	NE.	2 GL	N B	82	,	26.539	57.994	89.077	1.00 96.05
	10	2305	C	GL	N, B	82		23.906	54.677	86.585	1.00 99.75
		2306	0	GL	N B	82		24.310	53.753	87.293	1.00100.00
		2307	N	GL	UВ	83		22.683	55, 204	86.689	1.00100.00
		2308	CA	GL	UВ	83		21.697	54.743	87.665	1.00 98.86
		2309	СВ	GL	U B	83		20.397	55.543	87.519	0.00 99.32
	15	2310	CG	GL	U.B	83		20.554	57.043	87.717	0.00 99.30
		2311	CD	GĻΙ	UВ	83	•	21.051	57.409	89.104	0.00 99.42
		2312	OE	LGL	JВ	83		21.267	58.612	89.362	0.00 99.48
		2313	OE2	2 GL	JВ	83		21.225	56.495	.89.938	0.00 99.48
		2314	С	GL	JB	83		21.407	53.252	87.498	1.00 99.34
	20	2315	0	GLU	JВ	83		22.299	52.418	87.668	1.00 98.62.
		2316	N	VAI	В	84		20.163	52.920	87.156	1.00100.00
		2317	CA	VÀI	В	84		19.747	51.521	86.978	1.00100.00
		2318	CB	VAI		84		18.263	51,420	.86.471	1.00100.00
	~~	2319	CG1	VAI	В	84		17.268	51.796	87.589	1.00 99.23
	25	2320	CG2	VAL	В	84	• •	18.076	52.328	85.269	1.00100.00
		2321	С	VAL		84		20.645	50.721	86.012	1.00100.00
		2322	0	VAL		84		20.416	49.518	85.793	1.00100.00
		2323	N	LYS		85		21.667	51.379	85.454	1.00 96.27
	20	2324	CA	LYS		85		22.564	50.722	84.514	1.00 91.89
	30	2325	СВ	LYS		85		23.052	51.715	83.457	1.00 92.14
		2326	CG	LYS		85		23.655	51.051	82.243	0.00 91.98
		2327	CD	LYS		85		24.401	52.034	81.339	0.00 91.89
		2328	CE	LYS		85		25.031	51.302	80.154	0.00 91.77
	25	2329	NZ	LYS		85		25.878	52.209	79.338	0.00 91.53
•	35	2330	С	LYS		85		23.759	50.084	85.215	1.00 90.19
		2331	0	LYS		85		23.699	48.911	85.616	1.00 86.89
		2332	N	PHE		86		24.837	50.852	85.377	1.00 89.52
		2333	CA	PHE		86		26.035	50.321	86.019	1.00 88.74
,	10	2334	CB	PHE		86		27.275	51.138	85.641	1.00 92.15
-	40	2335	CG	PHE		86		27.777	50.850	84.253	1.00 98.73
		2336		PHE		86		27.403	51.658	83.178	1.00 99.74
		2337		PHE		86		28.594	49.744	84.009	1.00100.00
		2338	CE1	PHE	В	86		27.834	51.370	81.872	1.00100.00

	2339	e CE	E2 PF	HE E	86	29.031	49.442	82.709	1.00	0100.00
	2340) C2	Z Pi	IE E	86	28.649	50.259	81.637	7 1.00	0100.00
	2343	L C	PF	IE E	86	25.988	50.127	87.534	1.00	85.29
	2342	2 0	PF	IE E	86	26.644	49.219	88.051	1.00	84.94
5	2343	3 N	II	ΕE	87	25.232	50.955	88.252		80.15
	2344	C.A	II A	E E	87	25.134	50.789			75.10
	2345	CE	II	E E	87	24.651	52.075	90.395		73.06
	2346	CG	2 II	E B	87	24.352	51.792			72.58
	2347	CG	1 IL	E B	87	25.724	53.160	90.271		
10	2348	CD	1 IL	E B	87	25.436	54.404			70.71
	2349	С	IL	E B	87	24.199	49.632			72.87
	2350	0	IL	ЕВ	87	24.378	49.010			
	2351	N	ME	т в	88	23.203	49.343			
	2352	CA	ME	т в	88	22.297	48.233	89.537		68.05
15	2353	СВ	ME	т в	88	20.942	48.432	88.854		68.28
	2354	CG	ME	т в	88	20.012	49.364			66.92
	2355	SD	ME	т в	88	19.619	48.738	91.273		59.10
	2356	CE	ME	т в	88	18.028	49.538	91.593		67.20
	2357	С	ME:	гв	88	22.913	46.913	89.101		66.04
20	2358	0	ME:	r B	88	22.416	45.844	89.444		68.71
	2359	N	ASI	1 B	89	24.002	46.997	88.347		64.44
	2360	CA	ASI	1 B	89	24.719	45.817	87.884		62.80
	2361	СВ	ASI	1 В	89	25.225	46.019	86.456	1.00	70.00
	2362	CG	ASN	1 B	89	24.345	45.342	85.425		80.14
25	2363	OD1	. ASN	I B	89	23.142	45.618	85.326	1.00	85.25
٠,	2364	ND2	ASN	B	89	24.942	44.444	84.647	1.00	83.00
	2365	С	ASN	B	89	25.905	45.523	88.798	1.00	60.13
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20	2367	N	LEU	В	90	26.121	46.379	89.800	1.00	53.28
30	2368	CA	LEU	В	90	27.229	46.185	90.743	1.00	50.44
	2369	CB	LEU		90	27.522	47.473	91.534	1.00	48.07
	2370	CG	LEU		90	28.133	48.680	90.792	1.00	51.30
	2371		LEU		90	28.202	49.877	91.723	1.00	47.19
25	2372		LEU		90	29.517	48.346	90.261	1.00	47.85
35	2373	С	LEU		90	26.941	45.040	91.710	1.00	46.83
•	2374	0	LEU		90	27.834	44.256	92.032	1.00	44.52
	2375	N	PRO		91	25.691	44.929	92.196	1.00	46.91
	2376	CD	PRO		91	24.537	45.840	92.097	1.00	45.81
40	2377	CA	PRO		91	25.400	43.834	93.121	1.00	44.29
40	2378	СВ	PRO		91	23.910	43.997	93.377	1.00	47.92
	2379	CG	PRO		91	23.748	45.491	93.342	1.00	45.72
	2380	C	PRO		91	25.733	42.522	92.438	1.00	45.05
	2381	0	PRO	В	91	26.161	41.555	93.073	1.00	12.25

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	2598	3 0	ARG B 1	117		13.138	47.846	91.575	1.00	41.98
	2599	N	LEU B 1	118		13.904	46.636	93.284	1.00	34.54
	2600) CA	LEU B 1	118		15.086	46.207	92.541	1.00	35.55
5	2601	CB	LEU B 1	118		16.072	45.535	93.512	1.00	39.36
	2602	: CG	LEU B 1	118		16.690	46.395	94.623	1.00	32.09
	2603	CD	1 LEU B 1	118		17.269	45.487	95.670	1.00	30.29
	2604	CD	2 LEU B 1	118		17.745	47.337	94.041	1.00	30.17
	2605	C	LEU B 1	18		14.841	45.286	91.325	1.00	31.41
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•	2607	N	PRO B 1	.19		15.656	45.431	90.276	1.00	30.38
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	2609	CA	PRO B 1	.19		15.502	44.595	89.082	1.00	35.63
	2610	CB	PRO B 1	19		16.618	45.083	88.167	1.00	33.60
15	2611	CG	PRO B 1	19		16.783	46.514	88.585	1.00	32.98
	2612	С	PRO B 1	19		15.668	43.120	89.432	1.00	36.42
	2613	0	PRO B 1	19		16.320	42.759	90.415	1.00	34.89
	2614	N	LYS B 1	20		15.078	42.263	88.621	1.00	36.83
	2615	CA	LYS B 1	20		15.169	40.846	88.877	1.00	36.08
20	2616	CB	LYS B 1	20		14.562	40.090	87.710	1.00	35.56
	2617	CG	LYS B 1	20		14.383	38.610	87.966	1.00	38.99
	2618	CD	LYS B 1	20		14.017	37.915	86.665	1.00	40.22
	2619	CE	LYS B 1	20		14.047	36.418	86.838	1.00	34.37
	2620	NZ	LYS B 12	20		14.391	35.783	85.555	1.00	42.21
25	2621	С	LYS B 12			16.623	40.403	89.078	1.00	36.74
•	2622	0	LYS B 12			16.956	39.727	90.051	1.00	36.28
	2623	N	GLN B 12	21		17.482	40.810	88.156	1.00	35.29
	2624	CA	GLN B 12			18.886	40.428	88.176	1.00	38.60
20	2625	СВ	GLN B 12	21		19.570	40.985	86.935	1.00	41.25
30	2626	CG	GLN B 12			20.845	40.290	86.553	1.00	51.81
	2627	CD	GLN B 12			21.324	40.707	85.173	0.50	51.96
	2628		GLN B 12			21.199	41.871	84.783	0.50	53.41
	2629		GLN B 12			21.884	39.760	84.433	0.50	50.04
25	2630	С	GLN B 12			19.654	40.846	89.420	1.00	36.51
35	2631	0	GLN B 12		. (20.453	40.079	89.952	1.00	35.73
	2,632	N	THR B 12			19.422	42.055	89.900	1.00	38.81
	2633	CA	THR B 12			20.154	42.487	91.076	1.00	34.30
	2634	СВ	THR B 12			20.205	44.027	91.153	1.00	30.34
40	2635		THR B 12			19.300	44.497	92.140	1.00	41.29
40	2636	CG2				19.830	44.622	89.830	1.00	24.97
	2637	C	THR B 12				41.854	92.341	1.00	30.92
	2638	0	THR B 12			20.315		93.238	1.00	38.46
	2639	N	PHE B 12	3	1	18.254	41.692	92.417	1.00 2	29.82

	2640) CA	PHE	B 123	17.65	1 41.053	93.591	1.0	0 28.49
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	2643	CE	1 PHE.	B 123	15.034	41.084	95.767	1.0	0 38.16
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	2646	CE	2 PHE	B 123	14.432	38.360	95.592	1.0	0 34.78
	2647	CZ	PHE	B 123	14.025	39.081	96.714	1.00	0 37.18
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. 10	2649	0	PHE	B 123	18.194	39.017	94.720	1.00	32.37
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	2652	СВ	GLU	B 124	18.452	36.988	91.103	1.00	23.09
	2653	CG	GLU :	B 124	16.977	36.585	90.977	1.00	34.98
15	2654	CD	,GLU	B 124	16.628	35.990	89.627	1.00	38.90
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, .	2656	OE:	2 GLU 1	B 124	17.487	36.052	88.707	1.00	40.98
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20	2659	N		3 125	21.066	38.341	92.553	1.00	27.14
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	2661	СВ	ALA E		23.229	39.432	92.238	1.00	23.38
	2662	С	ALA E		22.563	38.411	94.438	1.00	32.42
~ -	2663	0	ALA E	125	23.241	37.627	95.113	1.00	35.19
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35	2674	CB	THR B		18.273	36.225	96.549	1.00	30.96
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5	6542	OE1	GLN	D	155		10.738	71.295	160.385	1.00	62.31
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	6554	CG	LEU	D	157		4.548	64.373	156.048	1.00	62.30
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	6556	CD2	LEU	D	157		4.680	64.525	154.562	1.00	67.25
20	6557	С	LEU	D	157		4.559	67.384	157.121	1.00	45.20
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25	6562	CG	LYS	D	158		3.185	68.983	161.581	1.00	41.48
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30	6567	0	LYS	D	158		2.475	70.166	158.404	1.00	49.43
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5	6671	N	ASP' D	173	1.632	70.876	144.382	1.00	49.47
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10	6676	OD2	ASP D	173 [.]	2.615	73.853	142.533	1.00	61.67
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25	6691	CG2	THR D	175	7.036	68.961	143.087	1.00	40.23
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35	6701	С	GLU D	176	11.802	67.948	146.695	1.00	30.62
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10	6934	СВ			205	29.314		158.681		34.86
	6935	CG			205	30.613		157.849		40.22
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15	6939	0			205	26.646		158.864		33.73
	6940	N			206	26.828		159.681		29.79
	6941	CA			206			159.673		30.19
	6942	СВ			206	24.767		160.950		30.10
	6943	CG			206	25.227		162.198		34.91
20	6944	CD			206	24.366		163.353		34.39
70	6945	NE			20.6	24.790		163.901		45.41
	6946	CZ			206	25.557		164.977		52.92
	6947				20.6			165.618		54.52
	6948		ARG		'	25.906		165.408		56.84
25	6949	C			206			159.542		33.05
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	6951	N			•	23.999		159.158		35.91
	6952	CA			207	23.713		158.913		37.61
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30	6954	.CG			207	22.238		157.242		41.56
	6955		LEU					158.467		
	6956		LEU			21.181				39.02
	6957	C			207	23.123		160.049		37.51
	6958	0	LEU			23.120		159.967		38.35
35	6959	N			208	22.628		161.092		24.15
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	6966	CA	ASN			19.231		160.961		21.42
	6967	CB								17.48
	0901	CD	ASN	ט	203	18.299	51.009	162.188	T.00	16.20

	6968	CG	ASN	D	209	16.963	58.515	161.987	1.00	19.86
	6969	OD1	ASN	D	209	16.486	58.700	160.868	1.00	14.67
	6970	ND2	ASN	D	209	16.347	58.895	163.092	1.00	17.14
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5	6972	0	ASN	D	209	19.303	60.280	161.302	1.00	14.34
	6973	N	PHE	D	210	21.001	59.368	160.170	1.00	18.04
	6974	CA	PHE	D	210	21.684	60.638	159.921	1.00	16.36
	6975	CB	PHE	D	210	23.180	60.484	160.149	1.00	19.10
	6976	CG	PHE	D	210	23.956	61.764	159.969	1.00	21.10
10	6977	CD1	PHE	D	210	23.655	62.874	160.727	1.00	14.31
•	6978	CD2	PHE	D	210	24.995	61.840	159.046	1.00	19.80
	6979	CE1	PHE	D	210	24.374	64.059	160.577	1.00	19.27
	6980	CE2	PHE	D	210	25.729	63.025	158.885	1.00	23.51
	6981	CZ	PHE	D	210	25.417	64.131	159.649	1.00	15.26
15	6982	С	PHE	D	210	21.446	61.061	158.470	1.00	15.01
	6983	0	PHE	D	210	21.847	60.364	157.552	1.00	18.32
	6984	N	LEU	D	211	20.776	62.193	158.282	1.00	17.17
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	6986	СВ	LEU	D	211	21.732	63.443	156.385	1.00	12.81
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	6989	CD2	LEU	D	211	21.342	65.654	157.563	1.00	8.25
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	6995	CB	PRO	D	212	17.088	59.420	156.148	1.00	19.76
	6996	CG	PRO	D	212	16.818	60.432	157.181	1.00	24.29
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	7003		TRP			14.125	64.013	151.149	1.00	19.97
	7004	CE2	TRP	D	213	14.126	64.962	150.091	1.00	20.58
	7005		TRP			13.012	63.182	151.315	1.00	14.88
	7006		TRP			16.056	65.151	151.198	1.00	15.78
40	7007		TRP			15.317		150.148	1.00	20.92
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	7009	CZ3	TRP	D	213	11.943	63.318	150.435	1.00	25.52
	7010	CH2	TRP	D	213	11.975	64.268	149.394	1.00	22.12

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25	7035		TYR D				145.396		25.39
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	7037		TYR D		21.159		144.213		22.79
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30	7040	ОН	TYR D		17.739		143.211		35.64
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	7043	N	SER D		24.706		148.708		21.01
25	7044	CA	SER D		26.066		149.147		19.51
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	7054	OE1	GLU D 2	19	31.111	57.021	146.460	1.00	31.78
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	7228	CG	LEU	D	240	43.448	59.840	148.254	1.00	48.36
	7229	CD1	LEU	D	240	43.935	60.902	147.270	1.00	52.77
5	7230	CD2	LEU	Ď	240	44.617	59.195	148.980	1.00	52.54
	7231	C.	LEU	D	240	40.354	59.860	148.207	1.00	38.95
	7232	0	LEU	D	240	40.218	59.698	146.991	1.00	40.40
	7233	N	ALA	D	241	39.809	59,052	149.113	1.00	35.76
	7234	CA	ALA	D	241	38.959	57.934	148.706	1.00	39.83
10	7235	СВ	ALA	D	241	38.469	57.149	149.931	1.00	34.80
	7236	С	ALA	D	241	37.761	58.474	147.918	1.00	38.65
	7237	0	ALA	D	241	37.354	57.887	146.921	1.00	44.66
	7238	N	TYR	D	242	37.202	59.593	148.369	1.00	37.78
	7239	CA	TYR	D	242	36.065	60.204	147.700	1.00	37.01
15	7240	СВ	TYR	D	242	35.650	61.476	148.424	1.00	30.63
	7241	CG	Τ̈́ΥR	D	242	34.652	62.300	147.646	1.00	28.13
	7242	CD1	TYR	D	242	33.292	62.048	147.741	1.00	30.93
	7243	CE1	TYR	D	242	32.366	62.823	147.052	1.00	31.95
	7244	CD2	TYR	D	242	35.072	63.349	146.832	1.00	32.54
20	7245	CE2	TYR	D	242	34.161	64.130	146.136	1.00	35.49
	7246	CZ	TYR	D	242	32.804	63.862	146.252	1.00	36.61
	7247	ОН	TYR	D	242	31.888	64.643	145.584	1.00	37.48
	7248	С	TYR	D	242	36.405	60.542	146.246	1.00	44.22
	7249	.0	TYR	D	242	35.595	60.324	145.333	1.00	42.91
25	7250	N	ASN	D	243	37.597	61.088	146.032	1.00	46.14
,	7251	CA	ASN	D	243	38.024	61.444	144.681	1.00	47.89
	7252	СВ	ASN	D	243	39.320	62.253	144.720	1.00	48.01
	7253	CG	ASN	D	243	39.078	63.723	145.003	1.00	50.35
	7254	OD1	ASN	D	243	39.816	64.355	145.758	1.00	51.70
30	7255	ND2	ASN	D	243	38.040	64.278	144.389	1.00	50.60
	7256	С	ASN	D	243	38.207	60.210	143.825	1.00	46.63
	7257	0	ASN	D	243	37.946	60.247	142.637	1.00	44.75
	7258	N	ARG	D	244	38.645	59.116	144.437	1.00	50.41
	7259	CA	ARG	D	244	38.849	57.869	143.714	1.00	55.73
35	7260	CB	ARG	D	244	39.581	56.855	144.592	1.00	58.07
*	7261	CG	ARG	D	244	41.077	56.769	144.384	1.00	66.11
	7262	CD	ARG	D	244	41.807	57.981	144.923	1.00	73.72
	7263	NE	ARG	D	244	43.230	57.696	145.119	1.00	81.74
	7264	CZ	ARG	D	244	43.708	56.796	145.980	1.00	83.33
40	7265	NH1	ARG	D	244	42.877	56.083	146.737	1.00	83.12
	7266	NH2	ARG	D	244	45.019	56.612	146.090	1.00	80.19
	7267	С	ARG	D	244	37.530	57.250	143.250	1.00	60.32
	7268	0	ARG	D	244	37.494	56.543	142.242	1.00	59.48

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	7312	OH2	RAW S	W :	22	30.959	61.833 94.884	1.00 26.91
	7313	ОН2	raw s	W	23	13.805	60.126 163.832	1.00 30.48
	7314	OH2	raw s	W	24	27.234	69.610 148.193	1.00 22.34
	7315	ОН2	raw s	W	25	18.824	60.189 114.266	1.00 23.07
5	7316	OH2	raw s	W	26	41.077	49.283 99.183	1.00 37.57
	7317	OH2	RAW S	W	27 '	10.572	28.703 137.018	1.00 37.26
	7318	OH2	RAW	W	28	16.340	75.164 175.623	1.00 27.57
	7319	OH2	raw s	W	29	23.460	60.770 117.115	1.00 26.41
	7320	OH2	RAW	W	30	40.206	58.426 156.934	1.00 32.69
10	7321	OH2	RAW	W	31	6.625	51.188 155.796	1.00 23.16
	7322	OH2	RAW	M	32	45.626	67.086 162.002	1.00 34.83
	7323	OH2	rAW	W	33	10.396	75.275 139.683	1.00 44.91
	7324	OH2	raw :	W	34	-0.601	31.861 146.272	1.00 24.79
	7325	OH2	WAT	W	35	17.494	70.622 152.608	1.00 24.54
15	7326	OH2	WAT	W	36	40.844	64.399 177.253	1.00 38.86
	7327	OH2	WAT	W	37	9.317	76.714 155.588	1.00 44.72
	7328	ОН2	WAT	W	38	27.274	48.442 122.282	1.00 49.70
	7329	ОН2	WAT	W	39	16.004	37.400 99.199	100 43.82
	7330	ОН2	WAT	W	40	12.464	57.862 103.307	1.00 25.85
20	7331	OH2	TAW	W	41	16.000	50.457 119.288	1.00 41.83
	7332	OH2	WAT	W	42	11.536	62.676 115.517	1.00 21.38
	7333	OH2	WAT	W	43	29.945	32.976 146.925	1.00 40.38
	7334	OH2	WAT	W	44	34.140	42.113 149.283	1.00 42.33
	7335	OH2	WAT	W	45	7.925	76.405 126.399	1.00 39.14
25	7336	OH2	WAT	W	46 .	18.170	61.725 111.986	1.00 20.89
	7337	OH2	WAT	W	47	30.755	77.804 153.505	1.00 19.49
	7338	OH2	TAW	W	48	41.754	57.323 159.509	1.00 50.17
	7339	OH2	TAW	M	49	0.432	34.807 151.800	1.00 32.45
	7340	OH2	TAW	W	50	7.115	42.218 141.155	1.00 44.48
30	7341	OH2	TAW	M	51	41.819	59.321 114.776	1.00 45.33
	7342		TAW			42.222	64.241 166.321	1.00 48.53
	7343		TAW		53	-2.402	32.063 152.567	
	7344		WAT			30.018		
0.5	7345		WAT			25.854	47.763 118.781	1.00 31.76
35	7346		WAT			29.404	29.191 146.912	1.00 39.21
	7347		TAW		57	7.137	64.606 107.354	1.00 35.06
	7348		WAT		58	30.727		1.00 54.96
	7349		TAW		59		28.876 101.654	1.00 35.31
40	7350		TAW		60		88.427 157.351	1.00 26.19
40	7351		TAW		61	27.419	47.353 95.987	1.00 57.79
	7352		TAW		62		48.522 96.797	1.00 54.20
	7353		TAW		63		84.485 164.897	
	7354	OH2	TAW	W	64	22.158	87.861 165.582	1.00 33.54

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                                                      1.00 34.16
     7397
          OH2 WAT W 107
                              34.830
                                      34.213 152.025
                                                      1.00 60.46
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	7398	OH2	WAT	W	108	13.929	50.264	161.908	1.00	38.42
	7399	OH2	WAT	W	109	7.928	47.573	126.723	1.00	61.79
	7400	ОН2	WAT	W	110	16.984	39.547	84.255	1.00	46.21
	7401	OH2	WAT	W	111	15.832	47.366	114.819	1.00	33.95
5	7402	OH2	WAT	W	112	13.984	73.451	167.234	1.00	54.71
	7403	OH2	WAT	W	113	9.368	43.081	92.878	1.00	24.54
	7404	OH2	WAT	W	114	-3.176	65.328	167.249	1.00	54.79
	7405	ОН2	TAW	W	115	10.815	55.601	163.806	1.00	36.83
	7406	OH2	WAT	W	116	15.643	54.415	93.626	1.00	56.57
10	7407	OH2	WAT	W	117	18.184	73.663	165.116	1.00	34.52
	7408	ОН2	WAT	W	118	5.305	83.283	114.524	1.00	25.41
	7409	OH2	WAT	W	119	32.518	33.657	139.051	1.00	49.90
	7410	OH2	WAT	W	120	17.065	74.471	161.007	1.00	49.07
	7411	OH2	WAT	W	121	33.595	77.512	125.281	1.00	50.88
15	7412	OH2	WAT	W	122	17.588	81.103	156.085	1.00	50.84
	7413	OH2	TAW	W	123	41.500	66.054	175.536	1.00	56.58
	7414	OH2	WAT	W	124	5.172	72.068	141.250	1.00	41.51
	7415	OH2	WAT	W	125	21.568	76.166	143.755	1.00	73.77
	7416	OH2	WAT	W	126	9.185	62.735	142.948	1.00	41.89
20	7417	OH2	TAW	M	127	34.832	65.837	107.513	1.00	45.85
	7418	OH2	WAT	W	128	7.851	35.881	155.165	1.00	39.11
	7419	OH2	TAW	W	129	22.684	74.042	102.458	1.00	46.57
	7420	OH2	TAW	W	130	27.459	69.125	104.582	1.00	38.96
	7421	OH2	WAT	W	131	-4.070	57.066	158.275	1.00	52.53
25	7422		TAW			28.752	47.213	86.649	1.00	58.61
	7423		WAT			24.922		178.645	1.00	45.28
	7424		WAT			33.981		155.674		30.59
	7425		TAW			14.099	•	139.548		46.13
20	7426		WAT			37.470		139.398		56.59
30	7427		WAT			38.013		158.862		44.49
	7428		TAW			42.958				
	7429				139	33.235		144.157		65.83
	7430		TAW			20.003		109.124		49.61
35	7431		WAT			41.759				
<i></i>	7432 7433		WAT			8.901		162.622		56.01
	7434		WAT		143	16.104		159.620		23.82
	7435		WAT					103.443		39.92
	7435		TAW					155.516		51.22
40	7437		WAT					124.194		54.32
70	7438		WAI			35.574		95.584 140.583		35.16
	7439				149	40.340				66.74
	7440		WAT			13.217		100.220		41.74
	7440	UIIZ	MAZZI	VV	100	13.41	. 50.504	100.592	1.00	48.44

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15.809 35.169 93.881
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           OH2 WAT W 152
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                                                       1.00 49.92
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                                       38.246 113.088
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                                                       1.00 42.46
     7456 OH2 WAT W 166
                               30.851 84.352 119.919
                                                       1.00 32.84
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                                                       1.00 26.48
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                                                       1.00 45.40
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                                                      1.00 28.83
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           OH2 WAT W 172
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                               2.228 80.152 121.569
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           OH2 WAT W 174
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                                                      1.00 76.14
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                                                      1.00 43.77
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          OH2 WAT W 181
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          OH2 WAT W 182
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          OH2 WAT W 184
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                                      29.149 169.017
                                                      1.00 59.49
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          OH2 WAT W 185
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          OH2 WAT W 192
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           OH2 WAT W 195
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           OH2 WAT W 196
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           OH2 WAT W 197
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     7488
           OH2 WAT W 198
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           OH2 WAT W 199
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           OH2 WAT W 200
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           OH2 WAT W 201
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           OH2 WAT W 202 .
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           OH2 WAT W 203
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                              15.407 67.707 145.749
                                                     1.00 57.01
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           OH2 WAT W 204
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           OH2 WAT W 205
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           OH2 WAT W 206
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                                                     1.00 25.64
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           OH2 WAT W 207
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          OH2 WAT W 208
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     7500
           OH2 WAT W 210
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     7501
           OH2 WAT W 211
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           OH2 WAT W 212
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     7503
           OH2 WAT W 213
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           OH2 WAT W 214
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           OH2 WAT W 215
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           OH2 WAT W 219
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           OH2 WAT W 221
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     7512 OH2 WAT W 222
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          OH2 WAT W 223
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                                     87.292 169.327
                                                     1.00 27.72
          OH2 WAT W 224
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          OH2 WAT W 225
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          OH2 WAT W 226
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          OH2 WAT W 227
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          OH2 WAT W 228
                             44.492
                                     73.582 159.662
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     7519
          OH2 WAT W 229
                             32.532 65.642 171.323
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     7520
          OH2 WAT W 230
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                                     41.490 138.172
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     7521
          OH2 WAT W 231
                             13.642
                                     56.805 126.904 1.00 40.69
     7522
          OH2 WAT W 232
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          OH2 WAT W 233
                             33.111
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                                                    1.00 54.29
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          OH2 WAT W 234
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                                     79.626 183.577
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     7525
          OH2 WAT W 235
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                                     63.753 113.280
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     7526
          OH2 WAT W 236
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                                     58.890 155.143
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	7527	ОН2	WAT	W	237	41.806	55.096 166.377	1.00 34.24
	7528	ОН2	WAT	W	238	21.432	37.843 88.704	1.00 44.13
	7529	ОН2	WAT	W	239	34.643	72.266 132.775	1.00 54.92
	7530	ОН2	WAT	W	240	35.338	85.572 172.058	1.00 53.95
5	7531	ОН2	WAT	W	241	16.256	49.306 116.927	1.00 31.04
	7532	OH2	WAT	W	242	41.709	64.265 169.935	1.00 38.19
	7533	OH2	WAT	W	243	28.757	83.671 179.021	1.00 53.65
	7534	ОН2	WAT	. M	244	38.413	67.817 108.876	1.00 52.81
	7535	ОН2	WAT	·W	245	20.663	64.332 111.428	1.00 38.62
10	7536	OH2	WAT	W	246	43.979	55.862 105.039	1.00 50.24
	7537	OH2	WAT	W	247	43.780	71.588 161.864	1.00 34.98
	7538	OH2	WAT	W	248	11.436	89.641 129.977	1.00 42.00
	7539	OH2	WAT	W	249	41.365	43.999 104.687	1.00 30.91
	7540	OH2	WAT	W	250	15.533	65.748 164.990	1.00 39.00
15	7541	OH2	WAT	W	251	42.846	65.656 89.632	1.00 43.71
	7542	OH2	TAW	W	252	21.227	58.593 112.048	1.00 35.62
	7543	OH2	WAT	W	253	5.127	90.024 111.033	1.00 52.52
	7544	OH2	WAT	W	254	35.042	73.905 117.216	1.00 44.07
	7545	OH2	TAW	W	255	18.017	23.723 142.245	1.00 67.41
20	7546	OH2	WAT	W	256	-1.547	33.928 137.556	1.00 47.00
	7547	OH2	WAT	W	257	10.061	75.671 157.442	1.00 55.48
	7548	он2	WAT	W	258	7.530	43.022 110.558	1.00 55.53
·	7549	OH2	TAW	W	259	26.307	46.356 121.321	1.00 52.54
	7550	OH2	WAT	W	260	37.686	38.689 95.823	1.00 44.59
25 [.]	7551	OH2	WAT	W	261	25.245	31.371 90.883	1.00 53.17
	7552		WAT			-4.652	34.436 142.767	1.00 43.66
	7553	OH2	WAT	W	263	40.945	75.530 172.545	1.00 55.53
	7554		TAW			-0.740	50.671 134.055	1.00 53.15
	7555		WAT			11.352	89.628 133.396	1.00 49.20
30	7556		WAT			37.290	34.588 109.736	1.00 50.49
	7557		WAT				37.013 101.903	
	7558		WAT				39.974 104.690	
	7559		WAT			0.643		1.00 40.99
25	7560		TAW			-4.940	•	1.00 31.26
35	7561		TAW				63.373 129.175	1.00 60.43
	7562		TAW			40.786	•	1.00 53.15
	7563		TAW			37.863	51.299 89.365	1.00 43.90
	7564		TAW				68.966 134.676	1.00 42.40
40	7565				275	11.659		1.00 43.46
40	7566		WAT			•	62.469 166.796	1.00 59.20
	7567		TAW				48.932 103.728	1.00 43.78
	7568		TAW				60.533 95.807	1.00 59.32
	7569	OH2	TAW	W	279	40.776	65.445 180.203	1.00 55.54

	7570	OH2	WAT	. W	280		-10.848	62.130	148.427	1.00	55.28
	7571	OH2	WAT	W	281		19.914	83.970	134.430	1.00	59.38
	7572	OH2	WAT	W	282		21.483	38.567	111.403	1.00	36.86
	75,73	OH2	WAŢ	W	2,83		38.967	62.592	110.346	1.00	60.29
5	7574	OH2	WAT	W	284		1.572	27.360	152,.361	1.00	37.17
	7575	OH2	TAW	W	285.		37.723	50.008	156.080	1.00	70.26
	7576	OH2	WAT	W	286		2.966	54.156	103.222	1.00	49.50
	7577	OH2	WAT	W	287		-1.589	50.288	102.705	1.00	73.77
	7578	OH2	WAT	. M	288		37.516	34.582	95.648	1.00	47.25
10	7579	OH2	WAT	W	289		18.845	80.053	161.444	1.00	58.39
	7580	OH2	WAT	· W	290		7.134	66.706	164.340	1.00	38.74
	7581	OH2	WAT	W	291		-5.751	62.419	111.073	1.00	38.80
	7582	OH2	WAT	W	292	•	28.331	79 ⁻ .237	149.230	1.00	45.26
	7583	OH2	TAW	W	293		28.736	72.020	170.198	1.00	50.37
15	7584	OH2	WAT	M	294.		7.807	53.256	124.651	1.00	35.93
	7585	OH2	WAT	W	295	,	5.276	73.692	117.621	1.00	48.57
	7586	ОН2	WAT	W	296		25.199	57.397	157.092	1.00	56.90
	7587	ОН2	WAT	W	297		23.531	47.649	123.560	1.00	48.49
	7588	OH2	TAW	W	298		22.536	36.594	112.333	1.00	38.66
20	7589	OH2	WAT	W	299	,	21.236	80.762	157.102	1.00	43.11
	7590	OH2	WAT	W	300		43.516	82.149	164.770	1.00	51.55
	7591	OH2	WAT	W	301		24.994	36.436	113.441	1.00	33.28
	7592		WAT	•			35.020	50.272	154.159	1.00	45.25
							19.366		119.490	1.00	44.24
25	7594				304			43.321	164.662	1.00	52.52
	7595				305		28.803	63.842	185.096	1.00	62.39
	7596		WAT				20.912	50.896	136.612	1.00	50.93
	7597		WAT				-0.130		157.579	1.00	59.19
20	7598		TAW				-3.536		123.927		52.36
30	7599		WAT				1.063		115.474		37.76
	7600						38.405				
					311				139.796		
	7602						17.857		169.577		59.11
25	7603				313		32.002				
35							12.387				
					315		0.891				
	7606						41.633		127.755		47.27
	7607		WAT				32.423		172.147		25.42
40							12.331		88.139		
40					319		15.441	•			
							40.548		157.210		43.00
	7611				321		22.089				
	7612	OH2	WA'I'	W	322		7.239	64.978	154.179	1.00	37.09

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     7622
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           OH2 WAT W 334
                                                     1.00 58.11
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           OH2 WAT W 335
                             23.195
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                                                     1.00 44.92
     7626 OH2 WAT W 336
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 15
                             15.464 66.982 107.609 1.00 26.03
     7627
           OH2 WAT. W 337
     7628
           OH2 WAT W 338
                             31.640 37.939 156.771
                                                     1.00 64.40
     7629 OH2 WAT W 339
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           OH2 WAT W 340
                             33.304 48.195 153.946
                                                     1.00 52.87
     7631 OH2 WAT W 341
                             -1.048 39.586 149.790
                                                     1.00 44.96
20
     7632 OH2 WAT W 342
                             35.287 57.004 186.624
                                                     1.00 52.61
     7633
           OH2 WAT W 343
                             2.662 60.413 144.348
                                                     1.00 57.31
     7634
           OH2 WAT W 344
                             14.848 52.164 166.291
                                                    1.00 42.67
     7635 OH2 WAT W 345 4.916 39,701 110.853 1.00 50.26
     7636
           OH2 WAT W 346
                             26.538 38.184 115.313
                                                    1.00 30.74
25
           OH2 WAT W 347 34.541 89.227 153.452
     7637
                                                    1.00 50.57
     7638
           OH2 WAT W 348
                             16.788 48.259 160.825
                                                    1.00 33.71
     7639
           OH2 WAT W 349
                            35.250 49.549 156.822
                                                    1.00 55.52
     7640
           OH2 WAT W 350
                             -3.272 54.762 155.638
                                                    1.00 42.76
     7641
           OH2 WAT W 351
                             26.550 78.335 147.072
                                                    1.00 48.38
30
     7642
          OH2 WAT W 352
                             32.287 29.392 98.163
                                                    1.00 26.70
     7643
          OH2 WAT W 353
                             34.002 66.690 112.543 1.00 45.32
     7644
           OH2 WAT W 354
                             0.508 65.282 103.717
                                                    1.00 52.50
     7645
          OH2 WAT W 355
                             4.524
                                                    1.00 56.33
                                     36.515 131.330
     7646
          OH2 WAT W 356
                             45.262
                                     59.545 161.086 1.00 41.72
35
     7647
          OH2 WAT W 357
                              4.961
                                     65.132 143.556
                                                    1.00 59.00
     7648
          OH2 WAT W 358
                             12.179 86.053 112.142
                                                    1.00 38.89
     7649
          OH2 WAT W 359
                            32.530 38.766 141.377
                                                    1.00 47.21
     7650
          OH2 WAT W 360
                              6.570 81.549 111.394
                                                    1.00 44.16
     7651
          OH2 WAT W 361
                             13.004
                                    72.367 165.279 1.00 45.96
40
     7652
          OH2 WAT W 362
                             31.973
                                    68.206 100.661 1.00 67.06
     7653
          OH2 WAT W 363
                             44.263
                                    51.590 120.936 1.00 54.89
    7654
          OH2 WAT W 364
                             30.071
                                    47.302 147.740
                                                    1.00 47.85
    7655
          OH2 WAT W 365
                             20.166 55.086 98.322 1.00 37.15
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7657 OH2 WAT W 367											
7658 OH2 WAT W 368		7656	OH2	WAT	W	366	15.595	43.155	106.386	1.00	66.70
7659 OH2 WAT W 369 20.753 88.034 127.140 5 7660 OH2 WAT W 370 9.041 55.783 142.925 7661 OH2 WAT W 371 26.451 83.995 180.936 7662 OH2 WAT W 372 33.378 81.968 123.649 7663 OH2 WAT W 373 7.117 59.500 167.632 7664 OH2 WAT W 375 39.406 42.629 92.387 7666 OH2 WAT W 375 39.406 42.629 92.387 7666 OH2 WAT W 376 -1.509 54.871 151.229 7667 OH2 WAT W 378 42.944 66.027 151.239 7669 OH2 WAT W 380 25.886 36.345 89.108 7671 OH2 WAT W 380 25.886 36.345 89.108 7671 OH2 WAT W 381 36.757 88.320 174.167 7672 OH2 WAT W 382 9.522 77.097 151.130 7673 OH2 WAT W 383 27.175 43.869 121.483 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 -2.133 41.763 107.962 7676 OH2 WAT W 386 17.581 68.108 147.353 7677 OH2 WAT W 387 -2.716 54.084 153.333 7678 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 399 32.478 44.660 97.842 25 7680 OH2 WAT W 399 32.478 44.660 97.842 25 7680 OH2 WAT W 391 49.539 60.328 164.723 7681 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7680 OH2 WAT W 399 19.586 57.647 152.990 7684 OH2 WAT W 399 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 399 31.233 30.782 96.006 36 OH2 WAT W 399 31.233 30.782 96.006 37691 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 19.392 60.601 89.688 7692 OH2 WAT W 400 19.392 60.601 89.688 7694 OH2 WAT W 400 19.392 60.601 89.688 7695 OH2 WAT W 400 19.392 60.601 89.688 7690 OH2 WAT W 400 19.392 60.601 89.688 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 19.392 60.601 89.688 7692 OH2 WAT W 400 19.392 60.601 89.688 7694 OH2 WAT W 400 19.392 60.601 89.688 7695 OH2 WAT W 400 19.392 60.601 89.688 7696 OH2 WA		7657	OH2	WAT	W	367	-3.446	69.862	164.261	1.00	46.11
5 7660 OH2 WAT W 370 9.041 55.783 142.925 7661 OH2 WAT W 371 26.451 83.995 180.936 7662 OH2 WAT W 372 33.378 81.968 123.649 7662 OH2 WAT W 373 7.117 59.500 167.632 7664 OH2 WAT W 374 -13.134 61.653 154.371 10 7665 OH2 WAT W 376 -1.509 54.871 151.229 7667 OH2 WAT W 377 2.526 67.268 166.696 7668 OH2 WAT W 377 2.526 67.268 166.696 7669 OH2 WAT W 378 42.944 66.027 151.239 7669 OH2 WAT W 379 -5.381 84.022 118.746 15 7670 OH2 WAT W 380 25.886 36.345 89.108 189.108 7671 OH2 WAT W 383 27.175 43.869 121.483 7671		7658	OH2	WAT	W	368	35.229	67.308	109.860	1.00	59.10
7661 OH2 WAT W 371		7659	ОН2	WAT	W	369,	20.753	88.034	127.140	1.00	46.69
7662 OH2 WAT W 372 33.378 81.968 123.649 7663 OH2 WAT W 373 7.117 59.500 167.632 7664 OH2 WAT W 374 -13.134 61.653 154.371 10 7665 OH2 WAT W 375 39.406 42.629 92.387 7666 OH2 WAT W 376 -1.509 54.871 151.229 7667 OH2 WAT W 377 2.526 67.268 166.696 7668 OH2 WAT W 378 42.944 66.027 151.239 7669 OH2 WAT W 379 -5.381 84.022 118.746 15 7670 OH2 WAT W 380 25.886 36.345 89.108 7671 OH2 WAT W 381 36.757 88.320 174.167 7672 OH2 WAT W 383 27.175 43.869 121.483 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 -2.133 41.763 107.962 7676 OH2 WAT W 386 17.581 68.108 147.353 7677 OH2 WAT W 388 1.214 58.353 145.206 7679 OH2 WAT W 388 1.214 58.353 145.206 7679 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 -0.526 39.840 108.033 7681 OH2 WAT W 391 49.539 60.328 164.723 7682 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 -5.305 81.386 124.897 7688 OH2 WAT W 396 -5.305 81.386 124.897 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 399 31.233 30.782 96.006 36 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 406 14.586 65.974 100.731	5	7660	OH2	WAT	W	370	9.041	55.783	142.925	1.00	48.36
7663 OH2 WAT W 373		7661	OH2	WAT	W	371	26.451	83.995	180.936	1.00	60.29
7664 OH2 WAT W 374 -13.134 61.653 154.371 10 7665 OH2 WAT W 375 39.406 42.629 92.387 7666 OH2 WAT W 376 -1.509 54.871 151.229 7667 OH2 WAT W 377 2.526 67.268 166.696 7668 OH2 WAT W 378 42.944 66.027 151.239 7669 OH2 WAT W 379 -5.381 84.022 118.746 15 7670 OH2 WAT W 380 25.886 36.345 89.108 7671 OH2 WAT W 381 36.757 88.320 174.167 7672 OH2 WAT W 382 9.522 77.097 151.130 7673 OH2 WAT W 383 27.175 43.869 121.483 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 -2.133 41.763 107.962 7676 OH2 WAT W 386 17.581 68.108 147.353 7677 OH2 WAT W 387 -2.716 54.084 153.333 7678 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 -0.526 39.840 108.033 7681 OH2 WAT W 391 49.539 60.328 164.723 7682 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 19.392 60.601 89.688 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7662	OH2	WAT	W	372	33.378	81.968	123.649	1.00	57.47
10 7665 OH2 WAT W 375		7663	OH2	WAT	W	373	7.117	59.500	167.632	1.00	54.66
7666 OH2 WAT W 376 7667 OH2 WAT W 377 7668 OH2 WAT W 377 7668 OH2 WAT W 378 7669 OH2 WAT W 379 7669 OH2 WAT W 379 7669 OH2 WAT W 380 7667 OH2 WAT W 380 7667 OH2 WAT W 380 7667 OH2 WAT W 381 7667 OH2 WAT W 381 7667 OH2 WAT W 382 7667 OH2 WAT W 382 7667 OH2 WAT W 383 7667 OH2 WAT W 383 7667 OH2 WAT W 384 7667 OH2 WAT W 384 7667 OH2 WAT W 385 7667 OH2 WAT W 385 7667 OH2 WAT W 385 7667 OH2 WAT W 386 7666 OH2 WAT W 386 7667 OH2 WAT W 386 7667 OH2 WAT W 386 7667 OH2 WAT W 387 7668 OH2 WAT W 388 7669 OH2 WAT W 389 7680 OH2 WAT W 389 7681 OH2 WAT W 390 7681 OH2 WAT W 391 7683 OH2 WAT W 392 7683 OH2 WAT W 393 7684 OH2 WAT W 394 7685 OH2 WAT W 395 7686 OH2 WAT W 396 7687 OH2 WAT W 396 7688 OH2 WAT W 396 7689 OH2 WAT W 396 7680 OH2 WAT W 396 7681 OH2 WAT W 391 7682 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 396 7686 OH2 WAT W 397 7686 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 400 19.392 OO.601 89.688 7691 OH2 WAT W 400 19.392 OO.601 89.688 7690 OH2 WAT W 400 19.392 OO.601 89.688 7691 OH2 WAT W 400 19.392 OO.601 89.688 7690 OH2 WAT W 400 19.392 OO.601 89.688		7664	OH2	WAT	W	374	-13.134	61.653	154.371	1.00	37.87
7667 OH2 WAT W 377 7668 OH2 WAT W 378 7669 OH2 WAT W 378 7669 OH2 WAT W 379 7669 OH2 WAT W 379 7669 OH2 WAT W 380 7670 OH2 WAT W 380 7671 OH2 WAT W 381 7671 OH2 WAT W 381 7672 OH2 WAT W 382 7673 OH2 WAT W 383 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 7676 OH2 WAT W 386 7677 OH2 WAT W 386 7677 OH2 WAT W 387 7678 OH2 WAT W 388 7677 OH2 WAT W 388 7678 OH2 WAT W 388 7679 OH2 WAT W 389 25.188 89.834 168.031 20 7675 OH2 WAT W 386 7677 OH2 WAT W 386 7677 OH2 WAT W 387 7678 OH2 WAT W 387 7678 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 7681 OH2 WAT W 391 7682 OH2 WAT W 391 7683 OH2 WAT W 392 7684 OH2 WAT W 394 30 7685 OH2 WAT W 394 30 7686 OH2 WAT W 395 7686 OH2 WAT W 395 7687 OH2 WAT W 396 7688 OH2 WAT W 397 7687 OH2 WAT W 398 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 7697 OH2 WAT W 406 14.586 65.974 100.731 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 406 14.586 65.974 100.731	10	7665	OH2	WAT	M	375	39.406	42.629	92.387	1.00	48.35
7668 OH2 WAT W 378 7669 OH2 WAT W 379 7669 OH2 WAT W 379 7669 OH2 WAT W 379 7670 OH2 WAT W 380 7671 OH2 WAT W 381 7672 OH2 WAT W 382 7673 OH2 WAT W 383 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 7676 OH2 WAT W 385 7677 OH2 WAT W 386 7677 OH2 WAT W 387 7678 OH2 WAT W 388 7677 OH2 WAT W 388 7678 OH2 WAT W 388 7679 OH2 WAT W 389 25.188 1.214 58.353 145.206 7679 OH2 WAT W 389 32.478 44.660 7679 OH2 WAT W 390 7681 OH2 WAT W 391 7682 OH2 WAT W 392 7683 OH2 WAT W 393 7684 OH2 WAT W 394 7685 OH2 WAT W 394 7686 OH2 WAT W 395 7686 OH2 WAT W 396 7687 OH2 WAT W 396 7687 OH2 WAT W 396 7688 OH2 WAT W 396 7689 OH2 WAT W 396 7689 OH2 WAT W 397 7680 OH2 WAT W 396 7680 OH2 WAT W 396 7681 OH2 WAT W 396 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 396 7686 OH2 WAT W 397 7686 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 7692 OH2 WAT W 401 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 406 14.586 65.974 100.731 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7666	OH2	WAT	W	376	-1.509	54.871	151.229	1.00	50.25
7669 OH2 WAT W 379		7667	OH2	WAT	W	377	2.526	67.268	166.696	1.00	68.89
15 7670 OH2 WAT W 380		7668	OH2	WAT	W	378	42.944	66.027	151.239	1.00	61.53
7671 OH2 WAT W 381		7669	OH2	WAT	W	379	-5.381	84.022	118.746	1.00	46.28
7672 OH2 WAT W 382 9.522 77.097 151.130 7673 OH2 WAT W 383 27.175 43.869 121.483 7674 OH2 WAT W 384 25.188 89.834 168.031 20 7675 OH2 WAT W 385 -2.133 41.763 107.962 7676 OH2 WAT W 386 17.581 68.108 147.353 7677 OH2 WAT W 388 1.214 58.353 145.206 7679 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 -0.526 39.840 108.033 7681 OH2 WAT W 391 49.539 60.328 164.723 7682 OH2 WAT W 392 -1.977 85.907 128.985 7683 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934	15	7670	OH2	WAT	W	380	25.886	36.345	89.108	1.00	44.82
7673 OH2 WAT W 383		7671	OH2	WAT	W	381	36.757	88.320	174.167	1.00	46.84
7674 OH2 WAT W 384		7672	OH2	WAT	W	382	9.522	77.097	151.130	1.00	49.50
20 7675 OH2 WAT W 385		7673	OH2	WAT	W	383	27.175	43.869	121.483	1.00	64.70
7676 OH2 WAT W 386 7677 OH2 WAT W 387 7678 OH2 WAT W 388 7678 OH2 WAT W 388 7679 OH2 WAT W 389 25 7680 OH2 WAT W 390 7681 OH2 WAT W 391 7682 OH2 WAT W 392 7683 OH2 WAT W 393 7684 OH2 WAT W 394 30 7685 OH2 WAT W 395 7687 OH2 WAT W 396 7688 OH2 WAT W 397 7688 OH2 WAT W 397 7689 OH2 WAT W 398 30 7689 OH2 WAT W 399 31.3851 30 7690 OH2 WAT W 399 31.233 30.782 30 OH2 WAT W 400 31 OH2 WAT W 401 31 OH2 WAT W 403 31 OH2 WAT W 404 40 OH4 S3.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7674	OH2	WAT	W	384	25.188	89.834	168.031	1.00	29.17
7677 OH2 WAT W 387 7678 OH2 WAT W 388 7679 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 7681 OH2 WAT W 391 7682 OH2 WAT W 392 7684 OH2 WAT W 394 30 7685 OH2 WAT W 395 7686 OH2 WAT W 396 7687 OH2 WAT W 397 7688 OH2 WAT W 397 7688 OH2 WAT W 397 7689 OH2 WAT W 399 31.233 30.782 7689 OH2 WAT W 399 35 7690 OH2 WAT W 400 7692 OH2 WAT W 401 7693 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 7696 OH2 WAT W 406 7697 OH2 WAT W 406 7697 OH2 WAT W 407 28.758 79.062 151.934	20	7675	OH2	WAT	W	385	-2.133	41.763	107.962	1.00	55.32
7678 OH2 WAT W 388 7679 OH2 WAT W 389 32.478 44.660 97.842 25 7680 OH2 WAT W 390 -0.526 39.840 108.033 7681 OH2 WAT W 391 49.539 60.328 164.723 7682 OH2 WAT W 392 -1.977 85.907 128.985 7683 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 399 31.233 30.782 96.006 368 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7676	OH2	WAT	W	386	17.581	68.108	147.353	1.00	50.43
7679 OH2 WAT W 389 25 7680 OH2 WAT W 390 7681 OH2 WAT W 391 7682 OH2 WAT W 392 7683 OH2 WAT W 393 7684 OH2 WAT W 394 30 7685 OH2 WAT W 395 7686 OH2 WAT W 396 7687 OH2 WAT W 397 7688 OH2 WAT W 398 7689 OH2 WAT W 399 31.233 30.782 7690 OH2 WAT W 400 7692 OH2 WAT W 402 7693 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 7696 OH2 WAT W 406 7697 OH2 WAT W 407 28.758 79.062 151.934		7677	OH2	WAT	W	387	-2.716	54.084	153.333	1.00	47.42
25 7680 OH2 WAT W 390		7678	OH2	WAT	W	388	1.214	58.353	145.206	1.00	54.87
7681 OH2 WAT W 391		7679	OH2	WAT	W	389	32.478	44.660	97.842	1.00	36.41
7682 OH2 WAT W 392 -1.977 85.907 128.985 7683 OH2 WAT W 393 19.586 57.647 152.990 7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 397 8.432 55.753 124.650 7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934	25	7680	OH2	WAT	W	390	-0.526	39.840	108.033	1.00	60.43
7683 OH2 WAT W 393		7681	OH2	WAT	W	391	49.539	60.328	164.723	1.00	48.42
7684 OH2 WAT W 394 10.485 50.231 124.846 30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 397 8.432 55.753 124.650 7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7682	OH2	WAT	W	392	-1.977	85.907	128.985	1.00	43.64
30 7685 OH2 WAT W 395 44.275 56.470 80.377 7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 397 8.432 55.753 124.650 7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7683	OH2	WAT	M	393	19.586	57.647	152.990	1.00	20.10
7686 OH2 WAT W 396 -5.305 81.386 124.897 7687 OH2 WAT W 397 8.432 55.753 124.650 7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7684	OH2	TAW	W	394	10.485	50.231	124.846	1.00	41.75
7687 OH2 WAT W 397 8.432 55.753 124.650 7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934	30	7685	OH2	TAW	M	395	44.275	56.470	80.377	1.00	45.96
7688 OH2 WAT W 398 13.851 49.974 119.218 7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7686	OH2	TAW	W	396	-5.305	81.386	124.897	1.00	42.75
7689 OH2 WAT W 399 31.233 30.782 96.006 35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7696 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7687	OH2	WAT	W	397	8.432	55.753	124.650	1.00	41.19
35 7690 OH2 WAT W 400 19.392 60.601 89.688 7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7688	OH2	WAT	M	398	13.851	49.974	119.218	1.00	31.25
7691 OH2 WAT W 401 21.499 64.661 106.290 7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7689	OH2	WAT	W	399	31.233	30.782	96.006	1.00	45.70
7692 OH2 WAT W 402 38.194 38.717 107.570 7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934	35	7690	OH2	WAT	W	400	19.392	60.601	89.688	1.00	52.10
7693 OH2 WAT W 403 19.114 46.019 85.421 7694 OH2 WAT W 404 40.014 53.000 88.531 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7691	OH2	TAW	W	401	21.499	64.661	106.290	1.00	56.95
7694 OH2 WAT W 404 40.014 53.000 88.531 3 40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934		7692	OH2	WAT	W	402	38.194	38.717	107.570	1.00	38.44
40 7695 OH2 WAT W 405 6.431 62.587 154.353 7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934							19.114	46.019	85.421	1.00	37.30
7696 OH2 WAT W 406 14.586 65.974 100.731 7697 OH2 WAT W 407 28.758 79.062 151.934			OH2	TAW	M	404	40.014	53.000	88.531	1.00	44.55
7697 OH2 WAT W 407 28.758 79.062 151.934	40	7695	OH2	TAW	W	405					39.93
											36.94
7698 OH2 WAT W 408 38.693 41.435 95.010		7697						79.062	151.934	1.00	37.27
		7698	OH2	WAT	W	408	38.693	41.435	95.010	1.00	57.50

7699 OH2 WAT W 409 25.591 57.948 93.946 1.00 45.44 7700 OH2 WAT W 410 27.357 55.891 95.673 1.00 63.85

END

PCT/US02/38715

Table IB
Atomic Coordinates of UPPS in complex with FPP

	C.R	YST1					.535 · 90	00 00		0 00
5						113.				
,		OM CD	<u>RESII</u> GLU A		X	100	Y	<u>Z</u> ,	<u>0cc</u>	<u>B</u> .
	1 2	CB CG	GLU A	14 14			26.564			
	3	CD					26.920			
	4	OE1	GLU A	•		477				67.15
10	5		GLU A GLU A	14		128		33.975		
10	6	C C	GLU A	14		370		34.921		
	7	0	GLU A	14		263	24.924			63.83
	8	N	GLU A	14		819				63.93
	9	CA	GLU A	14	•		24.367			67.24
15	10	N	VAL A				25.079			65.39
15	11	CA	VAL A				24.350			
	12	СВ	VAL A			.072				46.83
	13		VAL A				23.108			46.56
	14		VAL A				21.840			51.75
20	15	C	VAL A				22.773			
	16	0	VAL A			.330	23.654			43.02
	17	N	PRO A		•	.048	22.995			
	18	CD	PRO A							43.32
	19	CA	PRO A	16	,		25.08,6			
25		CB	PRO A	16		. 736 . 936	23.600 24.573			45.94
	21	CG	PRO A			. 389		•		46.50
	22	С	PRO A	16		.212	25.757 22.152			46.71
	23	0	PRO A	16		215	21.590	34.830 35.929		46.22
	24	N	THR A	17		607		33.713		44.84
30	25	CA	THR A	17		064		33.727		47.29
	26	СВ	THR A	17		170		32.879		43.32
	27		THR A	17		198	19.511	33.243		
	28		THR A				17.826			
	29	С	THR A	17		452	20.059	33.149		41.03
35	30	0	THR A	17		773	20.728	32.162		43.88
	31	N	GLN A	18		278	19.215	33.760		41.44
	32	CA	GLN A	18		614	19.000	33.231		41.88
	33	СВ	GLN A	18		348	17.893	33.993		46.62
	34	CG	GLN A	18		760	18.209	35.417		52.25
40	35	CD	GLN A	18		791	17.221	35.947		57.97
	36	OE1	GLN A	18			17.147	35.448		58.34
	37	NE2	GLN A	18			16.454	36.958		52.89
	38	С	GLN A	18			18.518	31.811		39.78
		•					229			

	39	0	GLN	A	18		4.495	17.642	31.603	1.00	34.46
	40	N	VAL	A	19		6.041	19.089	30.836	1.00	41.79
	41	CA	VAL	A	19		5.838	18.682	29.452	1.00	43.01
	42	CB	VAL	A	19	•	5.263	19.845	28.599	1.00	43.44
5	43	CG1	VAL	À	19	,	6.153	21.066	28,.705	1.00	47.93
	44	CG2	VAL	A	19		5.132	19.413	27.150	1.00	37.93
	45	С	VAL	A	19		7.143	18.184	28.837	1.00	41.23
	46	0	VAL	A	19		8.130	18.915	28.775	1.00	42.44
	47	N	PRO	A	20		7.162	16.922	28.373	1.00	40.76
10	48	CD	PRO	A	20	•	5.990	16.042	28.223	1.00	38.76
	49	CA	PRO	A	20		8.344	16.306	27.760	1.00	38.00
	50	СВ	PRO	A	20		7.797	14.993	27.198	1.00	36.72
	51	CG	PRO	A	20		6.338	15.287	26.983	1.00	35.57
	52	С	PRO	A	20		9.015	17.164	26.694	1.00	35,22
15	53	0	PRO	A·	20		8.363	17.638	25.771	1.00	32.45
	54	N	ALA	·A	21		10.323	17.354	26.830	1.00	30.30
	55	CA	ALA	A	21		11.079	18.157	25.882	1.00	23.48
	56	CB	ALA	A	21		12.369	18.617	26.524	1.00	21.08
	57	C	ALA	A	21		11.374	17.384	24.595	1.00	22.21
20	58	0	ALA	A	21		11.337	17.942	23.499	1.00	24.75
	59	. N	HIS	Α	22		11.687	16.101	24.739	1.00	22.28
	60	CA	HIS	A	22		11.961	15.241	23.597	1.00	23.83
	61	CB	HIS.	·A	22		13.429	14.815	23.561	1.00	17.45
	62	CG	HIS	Α	22		13.760	13.888	22.432	1.00	22.21
25	63	CD2	HIS	Α	22	• •	12.968	13.139	21.626	1.00	18.61
	64	ND1	HIS	A	22		15.054	13.650	22.020	1.00	22.86
	65	CE1	HIS	A	22		15.045	12.798	21.009	1.00	27.15
	66	NE2	HIS	A	22		13.791	12.471	20.750	1.00	23.08
	67	С	HIS	A	22		11.077	14.032	23.786	1.00	24.54
30	68	0	HIS	A	22		11.089	13.415	24.845	1.00	24.16
	69.	N	ILE	A	23		10.298	13.704	22.763	1.00	25.14
	70	CA	ILE	A	23		9.398	12.572	22.846	1.00	23.91
	71	CB	ILE	A	23		7.925	12.994	22.659	1.00	16.92
	72	CG2	ILE	A	23		7.035	11.765	22.660	1.00	16.92
35	73	CG1	ILE	A	23		7.495	13.927	23.797	1.00	16.92
	74	CD1	ILE	A	23		6.026	14.354	23.750	1.00	16.92
	75	С	ILE	A	23		9.714	11.516	21.818	1.00	25.13
	76	0	ILE	A	23		10.001	11.827	20.668	1.00	27.80
	77	N	GLY	A	24		9.663	10.261	22.254	1.00	25.44
40	78	CA	GLY		24		9.915	9.147	21.367	1.00	27.69
	79	С	GLY	A	24		8.578	8.514	21.053	1.00	29.71
	80	0	GLY	A	24		7.783	8.259	21.956	1.00	29.35
	81	N	ILE	A	25		8.306	8.275	19.777	1.00	29.96

	82	CA	ILE A	A 25	7.0	7.666	19.417	1.00	32.73
	83	CB	ILE A	A 25	6.1	.42 8.643	18.668	1.00	32.52
	84	CG2	ILE A	A 25	4.7	57 8.043	18.501	1.00	38.35
•	85	CG1	ILE A	25	6.0	9.948	19.446	1.00	29.69
5	86	CD1	ILE A	A 25	5.0	008 10.891	18.930	1.00	34.05
	87	С.	ILE A	A 25	7.2	09 6.436	18.555	1.00	34.24
	88	0	ILE F	A 25	7.8	01 6.497	17.478	1.00	40.45
	89	N	ILE F	A 26	6.6	95 5.315	19.052	1.00	32.06
	90	CA	ILE F	26	6.7	27 4.045	18.331	1.00	33.80
10	91	CB	ILE F	26	7.2	15 2.884	19.234	1.00	32.81
	92	CG2	ILE F	26	7.1	80 1.582	18.467	1.00	24.54
	93	CG1	ILE A	26	8.6	35 3.159	19.726	1.00	30.96
	94	CD1	ILE P	26	9.1	73 2.099	20.658	1.00	34.97
	95	С	ILE A	26	5.2	69 3.804	17.933	1.00	36.67
15	96	0	ILE A	26	4.4	68 3.302	18.734	1.00	33.26
	97	N	MET A	27	4.9	21 4.177	16.702	1.00	39.29
	98	CA	MET A	27	3.5	47 4.036	16.247	1.00	40.87
	99	СВ	MET A	27	3.2	21 5.071	15.159	1.00	36.66
	100	·CG	MET	A 2	7 4.	216 5.228	14.023	1.00	33.29
20	101	SD	MET	A 2	4.	359 6.996	13.573	1.00	28.20
	102	CE	MET	A 2	6.	102 7.183	13.528	1.00	29.62
	103	С	MET	A 2	3.	140 2.653	15.801	1.00	41.49
	104	0	MET	A 2	3.	772 2.041	14.937	1.00	44.33
,	105	N	ASP	A 28	2.	070 2.175	16.431	1.00	38.82
25	106	CA	ASP	A 28	1.	496 0.863	16.171	1.00	37.15
	107	CB	ASP	A 28	1.	780 -0.083	17.340	1.00	36.09
	108	CG	ASP .	A 28	3.	026 -0.902	17.131	1.00	37.61
	109	OD1	ASP	A 28	4.	123 -0.315	17.056	1.00	40.92
	110	OD2	ASP	A 28	2.	904 -2.139	17.031	1.00	43.44
30	111	С	ASP .	A 28	-0.	006 0.990	15.992	1.00	37.00
	112	0	ASP .	A 28	-0.	608 1.968	16.437	1.00	40.30
	113	N	GLY .	A 29	-0.	603 -0.001	15.339	1.00	32.98
	114	CA	GLY .	A 29	-2.0	0.013	15.128	1.00	31.71
	115	С	GLY .	A 29	-2.	440 0.281	13.694	1.00	34.52
35	116	0	GLY .	A 29	-3.	0.056	13.323	1.00	35.45
	117	N	ASN I	A 30	-1.9	0.762	12.886	1.00	35.21
	118	CA	ASN .	A 30	-1.	776 1.068	11.492	1.00	34.55
	119	CB	ASN I	A 30	-0.4	163 1.227	10.733	1.00	21.98
0	120	CG	ASN A	A 30	0.3	L73 2.589	10.951	1.00	23.62
40	121	OD1	ASN A	A 30	1.2	272 2.853	10.470	1.00	20.30
	122	ND2	ASN A	A 30	-0.5	3.465	11.670	1.00	20.74
	123	С	ASN A	A 30	-2.6	0.022	10.819	1.00	38.93
	124	0	ASN A	A 30	-3.7	787 .0.301	10.463	1.00	42.50

	125	N	GLY	Α	31		-2.111	-1.183	10.654	1.00	38.13
	126	CA	GLY	Α	31		-2.863	-2.253	10.014	1.00	37.44
	127	С	GLY	Α	31		-4.101	-2.713	10.768	1.00	37.86
	128	0	GLY	Α	31		-5.128	-3.027	10.172	1.00	33.07
5	129	N	ARG	Ά	32		-4.001	-2.769	12.089	1.00	41.86
	130	CA	ARG	Α	32		-5.119	-3.184	12.921	1.00	43.79
	131	СВ	ARG	A	32		-4.672	-3.236	14.384	1.00	50.98
	132	CG	ARG	A	32	,	-5.607	-3.971	15.326	1.00	67.82
	133	CD	ARG	Α	32		-5.003	-4.019	16.720	1.00	72.94
10	134	NE	ARG	A	32		-5.992	-4.324	17.750	1.00	79.64
	135	CZ	ARG	A	32		-5.790	-4.149	19.054	1.00	90.52
	136	NH1	ARG	A	32		-4.629	-3.672	19.490	1.00	100.13
	137	NH2	ARG	A	32		-6.750	-4.440	19.923	1.00	94.94
	138	С	ARG	A	32		-6.220	-2.150	12.721	1.00	41.07
15	139	0	ARG	··A	32		-7.386	-2.497	12.564	1.00	39.65
	140	N	TRP	A	33		-5.823	-0.880	12.716	1.00	39.29
	141	CA	TRP	Α.	33		-6.724	0.256	12.519	1.00	37.27
	142	CB	TRP	A	33		-5.924	1.559	12.530	1.00	28.51
	143	CG	TRP	A	33		-6.725	2.789	12.216	1.00	29.95
20	144	CD2	TRP	A	33		-6.861	3.421	10.939	1.00	34.19
	145.	CE2	TRP	A	33		-7.700	4.540	11.115	1.00	29.68
	146	CE3	TRP	A	33		-6.357	3.147	9.662	1.00	47.07
	147	CD1	TRP	A ·	33		-7.467	3.528	13.087	. 1.00	35.81
	148	NE1	TRP	Α	33		-8.055	4.583	12.436	1.00	31.40
25	149	CZ2	TRP	A	33		-8.048	5.390	10.059	1.00	27.96
	150	CZ3	TRP	Ά	33		-6.705	3.993	8.612	1.00	47.40
	151	CH2	TRP	A	33		-7.543	5.100	8.820	1.00	33.44
	152	С	TRP	A	33		-7.427	0.136	11.174	1.00	35.31
	153	0	TRP	A	33		-8.641	0.289	11.071	1.00	35.16
30	154	N	ALA	A	34		-6.639	-0.119	10.139	1.00	30.64
	155	CA	ALA	A	34		-7.164	-0.263	8.792	1.00	26.94
	156	CB	ALA	A	34		-6.012	-0.370	7.806	1.00	21.71
	157	С	ALA	A	34		-8.055	-1.499	8.689	1.00	29.54
	158	0	ALA	A	34		-9.206	-1.421	8.253	1.00	30.57
35	159	N	LYS	A	35		-7.509	-2.637	9.104	1.00	30.23
	160	CA	LYS	A	35		-8.218	-3.903	9.049	1.00	32.86
	161	CB	LYS	A	35		-7.350	-5.005	9.663	1.00	42.27
	162	CG	LYS	A	35		-7.354	-6.323	8.896	1.00	58.11
	163	CD	LYS	A	35		-6.766	-7.438	9.746	1.00	74.59
40	164	CE	LYS	A	35		-7.559	-7.597	11.042	1.00	85.25
	165	NZ	LYS	A	35		-6.948	-8.562	11.994	1.00	84.42
	166	С	LYS	A	35		-9.572	-3.845	9.754	1.00	38.17
	167	0	LYS	A	35		-10.486	-4.593	9.412	1.00	41.62

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1.00 41.65
                                         -2.956
                                                 10.730
                                -9.715
      168 N
               LYS A
                       36
                                                          1.00 43.49
                                         -2.859
                                                 11.445
      169
               LYS A
                       36
                               -10.980
           CA
                                                          1.00 52.09
                                        -2.303
                                                 12.859
      170
           СВ
               LYS A
                       36
                               -10.767
                                                          1.00 61.96
                                         -0.792
                                                 12.929
      171
           CG
               LYS A
                       36
                               -10.543
                                                          1.00 65.82
 5
                                         -0.276
                                                 14.383
      172
               LYS A
                               -10.483
           CD
                       36
                                                          1.00 62.88
                               -10.290
                                          1.253
                                                 14.449
      173
           CE
               LYS A
                       36
                                          1.809
                                                 15.840
                                                          1.00 66.92
      174
           NZ
               LYS A
                       36
                               -10.338
                                        -1.986
                                                 10.688
                                                          1.00 44.16
      175
           С
               LYS A
                       36
                               -11.975
                                                          1.00 46.34
               LYS A
                               -13.180
                                        -2.102
                                                 10.885
      176
           0
                       36
10
      177
           N
               ARG A
                               -11.473
                                         -1.119
                                                   9.816
                                                          1.00 44.81
                       37
                                         -0.237
                                                   9.049
                                                          1.00 46.91
      178
           CA
               ARG A
                               -12.340
                       37
                               -11.709
                                         1.145
                                                   8.899
                                                          1.00 54.16
      179
           CB
               ARG A
                       37
      180
           CG
               ARG A
                               -11.521
                                          1.863
                                                 10.211
                                                          1.00 51.20
                       37
      181
           CD
               ARG A
                               -10.928
                                          3.241
                                                 10.027
                                                          1.00 52.57
                       37
               ARG A
15
      182
           NE
                       37
                               -10.378
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                                                 11.289
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	212	N	ARG	Α	41	-5.222	-3.129	4.656	1.00	44.90
	213	CA	ARG	Α	41	-4.293	-3.028	5.765	1.00	46.18
	214	СВ	ARG	A	41	-3.560	-4.366	5.912	1.00	48.57
5	215	CG	ARG	Α	41	-2.470	-4.443	6.982	1.00	54.03
	216	CD.	ARG	A	41	-1.621	-5.703	6.774	1.00	54.03
	217	NE	ARG	A	41	-1.919	-6.838	7.664	1.00	58.63
	218	CZ	ARG	А	41	-3.134	-7.268	8.024	1.00	55.36
	219	NH1	ARG	А	41	-4.237	-6.661	7.596	1.00	56.78
· 10	220	NH2	ARG	A	41	-3.248	-8.344	8.799	1.00	41.95
	221	С	ARG	A	41	-3.294	-1.907	5.474	1.00	49.28
	222	0	ARG	A	41	-2.985	-1.085	6.338	1.00	51.60
	223	N	VAL	A	42	-2.819	-1.867	4.235	1.00	46.21
	224	CA	VAL	A	42	-1.823	-0.889	3.802	1.00	45.66
15	· 225 ·	CB	VAL	A	42	-1.361	-1.228	2.344	1.00	36.84
	226	CG1	VAL	A	42	-2.084	-0.351	1.340	1.00	30.96
	227	CG2	VAL	A	42	0.155	-1.107	2.221	1.00	31.91
	228	С	VAL	A	42	-2.214	0.604	3.915	1.00	49.01
	229	0	VAL	A	42	-1.341	1.467	4.028	1.00	53.47
20	230	N	PHE	A	43	-3.508	0.915	3.887	1.00	46.72
	231	CA	PHE	A	43	-3.942	2.311	4.002	1.00	44.27
	232	СВ	PHE	A	43	-5.458	2.448	3.827	1.00	37.66
,	233	CG	PHE	A	43	-5.920	2.446	2.397	1.00	36.94
	234	CD1	PHE	A	43	-5.009	2.523	1.345	1.00	36.78
25	235	CD2	PHE	A	43	-7.283	2.383	2.102	1.00	39.68
	236	CE1	PHE	A	43	-5.450	2.534	0.020	1.00	29.77
	237	CE2	PHE	A	43	-7.731	2.395	0.785	1.00	31.31
	238	CZ	PHE	A	43	-6.813	2.470	-0.258	1.00	29.07
	239	С	PHE	A	43	-3.583	2.844	5.375	1.00	46.39
30	240	0	PHE	A	43	-3.142	3.987	5.512	1.00	46.33
	241	N	GLY	A	44	-3.798	2.001	6.385	1.00	46.54
	242	CA	GLY	A	44	-3.512	2.362	7.763	1.00	43.50
	243	С	GLY	A	44	-2.251	3.185°	7.894	1.00	40.10
	244	0	GLY	A	44	-2.189	4.130	8.681	1.00	40.32
35 ⁻	245	N	HIS	A	45	-1.242	2.823	7.114	1.00	33.52
	246	CA	HIS	A	45	0.015	3.539	7.133	1.00	30.60
	247	CB	HIS	A	45	1.029	2.821	6.252	1.00	16.92
	248	CG	HIS	A	45	1.469	1.501	6.803	1.00	28.29
	249	CD2	HIS	A	45	2.701	0.954	6.934	1.00	34.82
40	250	ND1	HIS	A	45	0.582	0.560	7.277	1.00	34.82
	251	CE1	HIS	A	45	1.247	-0.511	7.675	1.00	39.36
	252	NE2	HIS	A	45	2.536	-0.297	7.477	1.00	40.10
	253	С	HIS	A	45	-0.169	4.986	6.686	1.00	34.04

	254	0	HIS	A	45		0.362	5.893	7.321	1.00	33.04
	255	N	LYS	A	46		-0.918	5.226	5.613	1.00	37.67
	256	CA	LYS	A	46		-1.112	6.606	5.190	1.00	36.56
	257	СВ	LYS	A	46		-2.029	6.714	3.981	1.00	27.77
5	258	CG	LYS	A	46		-2.167	8.154	3.490	1.00	36.67
	259	CD	LYS	A	46		-2.906	8.248	2.160	1.00	47.11
	260	CE	LYS	A	46	•	-2.187	7.465	1.060	1.00	45.30
	261	NZ	LYS	Α	46		-2.935	7.463	-0.231	1.00	54.67
	262	С	LYS	À	46		-1.737	7.348	6.350	1.00	35.24
10	263	0	LYS	Α	46		-1.280	8.429	6.723	1.00	34.48
	264	N	ALA	À	47		-2.781	6.757	6.924	1.00	34.22
	265	CA	ALA	A	47		-3.462	7.358	,8.069	1.00	33.65
	266	СВ	ALA	A	47		-4.588	6.451	8.550	1.00	22.25
	267	С	ALA	. A	47		-2.457	7.601	9.201	1.00	33.26
15	268	0	ALA	A	47		-2.505	8.632	9.876	1.00	35.94
	269	N	GLY	Α	48		-1.558	6.643	9.413	1.00	31.73
	270	CA	GLY	Α	48		-0.562	6.814	10.443	1.00	31.22
	271	С	GLY	Α	48		0.056	8.162	10.156	1.00	28.17
	272	0	GLY	A	48		0.063	9.050	11.005	1.00	30.21
20	273	N	MET	A	49		0.546	8.321	8.933	1.00	26.41
	274	CA	MET	A	49		1.168	9.565	8.510	1.00	26.13
	275	CB	MET	Α	49		1.525	9.501	7.019	1.00	26.11
	276	CG	MET	Α,	49		1.999	10.831	6.415	1.00	31.14
	277	SD	MET	A	49	, ,	2.596	10.723	4.688	1.00	30.86
25	278	CE	MET		49	0.1	1.149	10.009	3.871	1.00	27.72
	279	С	MET	Α	49		0.267	10.764	8.780	1.00	26.86
	280	0	MET	A	49		0.740	11.812	9.209	1.00	25.74
-	281	N	GLU	A	50		-1.028	10.621	8.532	1.00	26.86
•	282	CA	GLU		50		-1.943	11.725	8.780	1.00	29.13
30	283	CB	GLU,		50		-3.364	11.333	8.397	1.00	35.38
	284	CG	GLU		50		-3.465	10.916	6.948	1.00	42.20
	285	CD	GLU		50		-4.615			1.00	55.85
	286		GLU		50		-4.707		6.279	1.00	54.70
25	287		GLU		50		-5.414			1.00	62.59
35	288	С	GLU		50		-1.885	•	10.246	1.00	33.72
	289	0	GLU		50		-1.701		10.566		40.50
	290	N	ALA		51		-2.031		11.143	1.00	30.97
	291	CA	ALA		51		-1.972		12.560	1.00	29.01
40	292	CB	ALA		51		-2.288		13.384		33.60
40	293	C	ALA		51		-0.587	12.009	12.910		28.16
	294	0	ALA		51		-0.448		13.835		28.15
	295	N	LEU		52		0.439		12.182		26.73
	296	CA	LEU	A	52		1.785	12.051	12.475	1.00	26.65

	297	СВ	LEU	A	52		2.809	11.478	11.499	1.00	16.92
	298	CG	LEU	Α	52		4.267	11.370	11.979	1.00	16.92
	299	CD1	LEU	A	52		5.184	11.281	10.768	, 1.00	16.92
	300	CD2	LEU	Α	, 5Ż	•	4.661	12.570	12.823	1.00	22.52
5	301	С	LEU	·A	5,2		1.765	13.561	12.338	1.00	32.69
	302	0	LEU	Α	52	٠.,	2.309	14.273	13.180	1.00	34.28
	303	N	GLN	A	53		1.124	14.041	11.272	1.00	32.34
•	304	ĆA	GLN	Α	53		1.016	15:475	11.005	1.00	28.24
	305	СВ	GLN	A	53		0.241	15.729	9.714	1.00	22.43
10	306	CG	GLN	Ą	53		0.219	17.194	9.297	1.00	16.92
	307	CD	GLN	A	53		1.467	17.602	8.535	1.00	16.92
	308	OE1	GLN	A	53		2.512	16.956	8.631	1.00	26.60
	309	NE2	GLN	A	53		1.364	18.685	7.779	1.00	16.92
	310	С	GLN	A	53		0.302	16.180	12.150	1.00	31.47
15	311	0	GLN	A	53	•	0.740	17.227	12.618	.1.00	30.88
	312	N	THR	A	54	•	-0.809	15.598	12.583	1.00	32.71
	313	CA	THR	A.	54		-1.599	16.137	13.679	1.00	29.40
	314	CB	THR	A	54		-2.824	15.282	13.932	1.00	22.85
	315	OG1	THR	A	54		-3.692	15.346	12.796	1.00	33.45
20	316	CG2	THR	A	54		-3.545	15.751	15.186	1.00	16.92
	317	С	THR	A	54		-0.819	16.176	14.977	1.00	32.23
	318	0	THR	A	54		-0.781	17.197	15.652	1.00	35.38
	319	Ņ	۷AĻ	A	55,		-0.219	15.049	15.337	1.00	33.35
	320	CA	VAL	A	55		0.552	14.958	16.568	1.00	32.18
25	321	CB	VAL	A	55	• •	1.029	13.501	16.835	1.00	26.17
	322	CG1	VAL	Α	55		1.962	13.460	18.026	1.00	16.92
	323	CG2	VAL	A	55		-0.164	12.606	17.105	1.00	28.32
	324	С	VAL	A	55		1.760	15.875	16.514	1.00	32.33
	325	0	VAL	A	55		1.981	16.666	17.429	1.00	31.60
30	326	N	THR	A	56		2.531	15.773	15.435	1.00	31.81
	327	CA	THR		56		3.732	16.582	15.266	1.00	36.75
	328	СВ	THR		56		4.422	16.248	13.924	1.00	33.23
	329	OG1	THR	A	56		5.715	16.861	13.877	1.00	35.26
	330	CG2	THR		56		3.599	16.758	12.764	1.00	48.73
35	331	С	THR	A	56		3.416	18.082	15.341	1.00	40.46
	332	0	THR	A	56		4.227	18.881	15.801	1.00	43.12
	333	N	LYS		57		2.222	18.450	14.897	1.00	42.26
	334	CA	LYS		57		1.774	19.838	14.907	1.00	43.45
	335	CB	LYS	A	57		0.629	19.988	13.907	1.00	47.22
40	336	CG	LYS		57		0.464	21.352	13.292		47.96
	337	CD	LYS		57		-0.497	21.262	12.116		49.91
	338	CE	ĻYS		57		-1.823	20.642	12.534		55.23
	339	NZ.	LYS	A	57		-2.759	20.430	11.394	1.00	63.19
		•									

	340	С	LYS	7\	57	1.301	20.167	16.324	1.00 44.75
	341	0	LYS		57	1.783		16.955	1.00 48.17
	342	N	ALA		58	0.359		16.819	1.00 44.02
	343	CA	ALA		58	-0.174		18.158	1.00 45.02
5	344	CB	ALA		58	-1.048		18.520	1.00 31.05
_	345	C	ALA		58	0.957		19.165	1.00 45.60
	346	0	ALA		58	0.940		20.028	1.00 47.49
	347	Ŋ	ALA		59	1.941		19.046	1.00 43.55
	348	CA	ALA		59	3.085		19.948	1.00 44.39
10	349	СВ	ALA		59	3.934		19.682	1.00 36.73
	350	С	ALA		59	3.931		19.802	1.00 48.03
	351	0	ALA		59	4.663	,	20.714	1.00 49.73
	352	N	ASN		60	3.830		18.646	1.00 50.14
	353	CA	ASN		60	4.599		18.380	1.00 50.72
15	354	СВ	ASN		60	4.661	22.151	16.870	1.00 56.81
	355	CG	AŚN	A	60	5.519	23.346	16.516	1.00 59.09
	356	OD1	ASN	A	60	6.699	23.405	16.855	1.00 50.39
·	357	ND2	ASN	A	60	4.927	24.306	15.820	1.00 68.87
	358	C,	ASN	Α	60	3.998	23.099	19.095	1.00 48.92
20	359	0	ASN	Α	60	4.729	23.925	19.648	1.00 49.57
	360	N	LYS	A	61	2.668	3 23.189	19.091	1.00 44.16
	361	CA	LYS	A	61	1.978	24.296	19.739	1.00 42.23
	362	СВ	LYS	A,	61	0.494	24.296	19.378	1.00 38.81
•	363	CG	LYS	A	61	-0.376	23.520	20.360	1.00 49.61
25	364	CD	LYS	A	61	-1.847	23.893	20.228	1.00 61.71
,	365	CE	LYS	Α	61	-2.674	23.282	21.355	1.00 76.26
	366	NZ	LYS.	A	61	-4.111	23.687	21.306	1.00 77.30
	367	С	LYS	A	61	2.105	24.171	21.247	1.00 41.26
	368	0	LYS	A	61	1.872	25.120	21.987	1.00 38.34
30	369	N	LEU	A	62	2.470	22.982	21.697	1.00 43.33
	370	CA	LEU	A	62	2.598	3 22.724	23.117	1.00 40.43
	371	CB	LEU	A	62	2.047	21.331	23.436	1.00 41.05
	372	CG	LEU	A	62	1.512	21.076	24.843	1.00 43.45
	373		LEU		62	0.465		25.216	1.00 49.97
35	374	CD2	LEU	Α	62	0.909		24.888	1.00 41.95
	375	С	LEU	Α	62	4.043		23.572	1.00 37.78
	376	0	LEU		62	4.361		24.721	1.00 36.77
	377	N	GLY		63	4.919		22.662	1.00 34.00
	378	CA	GLY		63	6.310		23.026	1.00 34.47
40	379	С	GLY		63	7.250		23.130	1.00 34.70
	380	0	GLY		63	8.370		23.623	1.00 37.15
	381	N	VAL		64	6.830		22.703	1.00 32.50
	382	CA	VAL	A	64	7.745	19.951	22.764	1.00 33.85

	383	CB	VAI	A	64	7.075	18.672	22.254	1.00	38.31
	384	CG1	L VAI	A	64	8.104	17.563	22.102	1.00	45.70
	385	CG2	VAI	A	64	5.981	18.254	23.216	1.00	30.49
	386	С	VAI	A	64	8.923	20,305	21.861	1.00	32.11
5	387	0	VAI	A	64	8.738	20.626	20.693	1.00	35.71
	388	N	LYS	A	65	10.133	20.264	22.398	1.00	30.11
	389	CA	LYS	A	65	11.301	20.604	21.598	1.00	32.19
	390	СВ	LYS	A	65	12.555	20.633	22.464	1.00	34.45
	391	CG	LYS	A	65	13.133	22.024	22.668	1.00	28.19
· 10	392	CD	LYS	A	65	12.183	22.927	23.451	1.00	32.70
	393	CE	LYS	Α	65	12.850	24.251	23.841	1.00	50.92
	394	NZ	LYS	Α	65	14.038	24.082	24.743	1.00	60.18
	395	С	LYS	Α	65	11.542	19.683	20.411	1.00	32.24
	396	0	LYS	Α	65	11.799	20.154	19.307	1.00	32.31
15	397.	N	VAL	Α	66	11.466	18.374	20.634	1.00	29.19
	398	CA	VAL	Α	66	11.695	17.399	19.561	1.00	27.66
	399	СВ	VAL	Α	66	13.232	17.130	19.391	1.00	30.38
	400	CG1	VAL	A	66	13.926	17.314	20.720	1.00	29.01
	401	CG2	VAL	Α	66	13.498	15.717	18.840	1.00	16.92
20	402	С	VAL	A	66	10.970	16.069	19.763	1.00	22.57
	403	0	VAL	A	66	10.605	15.725	20.879	1.00	18.50
	404	N	ILE	A	67	10.730	15.346	18.670	1.00	23.89
,	405	CA	ILE	A	67	10.099	14.028	18.744	1.00	3124
	406	CB	ILE	A	67	8.541	14.075	18.622	1.00	30.49
25	407	CG2	ILE	A	67	7.963	14.971	19.709	1.00	32.00
	408	CG1	ILE	Α	67	8.113	14.561	17.242	1.00	35.49
	409	CD1	ILE	A	67	6.610	14.613	17.079	1.00	44.48
	410	С	ILE	A	67	10.671	13.104	17.674	1.00	32.32
	411	0	ILE	Ą	67	10.849	13.495	16.512	1.00	36.35
30	412	N	THR	A	68	10.988	11.885	18.100	1.00	27.06
	413	CA	THR	A	68	11.554	10.866	17.229	1.00	22.58
	414	CB	THR	A	68	12.836	10.287	17.823	1.00	20.26
	415	OG1	THR		68	13.811	11.331	17.956	1.00	31.06
	416	CG2	THR	A	68	13.373	9.182	16.937	1.00	16.92
35	417	С	THR		68	10.540	9.750	17.040	1.00	26.08
	418	0	THR		68	10.226	9.008	17.969	1.00	28.24
	419	N	VAL		69	10.028	9.657	15.818	1.00	25.72
	420	CA	VAL	A	69	9.022	8.677	15.450	1.00	22.44
	421	CB	VAL		69	8.025	9.297	14.488	1.00	20.89
40	422		VAL		69	7.234	10.378	15.180	1.00	16.92
	423		VAL		69	8.770	9.892	13.313	1.00	16.92
	424	С	VAL		69	9.667	7.490	14.770	1.00	23.00
	425	0	VAL	A	69	10.401	7.652	13.794	1.00 2	23.85

				_					15 205	1 00	25 00
	426	N	TYR		70		9.399 9.943	6.299 5.066	15.295 14.727		25.89 26.71
	427	CA	TYR		70				'		
	428	CB	TYR		70		9.802		15.728		22.08
_	429	CG	TYR		70		10.817	2.805	15.552		16.92
5	430	CD1	TYR	•	70		11.756	2.842			16.92
	431	CE1	TYR		70 ·		12.708	1.834	14.374		16.92
	432	CD2	TYR		70		10.856	1.723	16.440		18.76
	433	CE2	TYR		70		11.802			•	20.19
	434	CZ	TYR	A	70	'	12.723	0.774	15.272		23.85
10	435	OH	TYR	A	70		13.660	-0.218	15.136	1.00	28.88
	436	С	TYR	A'	70		9.150	4.752	13.454		27.42
	437	0	TYR	Α	70		8.125	4.053	1,3.508	1.00	29.24
•	438	N	ALA	A	71		9.640	5.272	12.324	1.00	26.20
	439	CA	ALA	A	71		9.004	5.115	11.013	1.00	27.77
15	440	СВ	ALA	A	71 ·		9.336	6.326	10.149	1.00	21.40
	441	С	ALA	Α	71		9.302	3.821	10.232	1.00	33.28
	442	0	ALA,	A	71		8.441	3.314	9.513	1.00	35.06
	443	N	PHE	A	72		10.514	3.292	10.344	1.00	34.13
	444	CA	PHE	A	72 .		10.837	2.055	9.640	1.00	35.25
20	445	СВ	PHE	A	72		11.105	2.336	8.152	1.00	28.54
	446	CG	PHE	Α	72		11.098	1.096	7.289	1.00	32.61
	447	CD1	PHE	Α	72		9.897	0.518	6.880	1.00	33.56
	448	CD2	PHE	Α,	72		12.290	0.478	6.917	1.00	35.80
	449	CE1	PHE	Α	72 " "	٠.	9.885	-0.661	6.113	1.00	28.42
25	450	CE2	PHE	A	7,2		12.283	-0.698	6.154	1.00	32.48
	451	CZ	PHE	Α	72		11.077	-1.265	5.753	1.00	31.11
	452	С	PHE	A	72		12.053	1.386	10.275	1.00	40.63
	453	0	PHE	A	72		13.172	1.865	10.135	1.00	43.32
•	454	N	SER	A	73		11.832	0.280	10.980	1.00	47.02
30	455	CA	SER	A	73		12.932	-0.435	11.627	1.00	49.68
	456	СВ	SER	A	73		12.409	-1.381	12.708	1.00	43.74
	457	OG	SER	A	73		12.032	-2.624	12.145	1.00	33.26
	458	С	SER	A	73		13.703	-1.250	10.601	1.00	52.36
	459	0	SER	Α	73		13.227	-1.477	9.487	1.00	53.00
35	460	N	THR	A	74		14.893	-1.697			57.20
•	461	CA	THR		74		15.726				62.04
	462	СВ	THR	A	74			-2.742	10.714	1.00	67.14
	463	OG1	THR		74			-1.557		1.00	74.37
	464		THR		74			-3.103			71.77
40	465	С	THR		74		15.027				62.95
	466	0.	THR		74			-4.441			62.39
	467	N	GLU		75			-4.252			63.63
	468	CA	GLU		75			-5.525			66.15
	-00	···	0.00	- 1	, 5			5.525	10.700	±.00	JJ. 1J

	469	СВ	GLU	Α	75	13.387	-6.084	12.203	1.00 75.90
	470	CG	GLU	Α	75	12.911	-7.521	12.255	1.00 93.53
	471	CD	GLU	Α	75	12.685	-8.000	13.669	1.00103.81
	472	OE1	GLU	A	75	11.907	-7.347	14.399	1.00110.70
5	473	OE2	GLU	Α	75	13.283	-9.030	14.048	1.00111.36
	474	c ·	GLU	Α	75	12.193	-5.457	10.096	1.00 66.40
	475	0	GLU	Α	75	11.395	-6.390	10.193	1.00 68.91
	476	N	ASN	Α	76	11.925	-4.362	9.393	1.00 64.57
	477	CA	ASN	Α.	76	10.646	-4.222	8.702	1.00 59.63
10	478	СВ	ASN	Α	76	10.136	-2.778	8.788	1.00 53.70
	479	CG	ASN	Α	76	9.370	-2.506	10.066	1.00 46.89
	480	OD1	ASN	Α	76	8.523	-3.299	10.470	1.00 50.66
	481	ND2	ASN	A	76	9.652	-1.377	10.700	1.00 40.20
	482	С	ASN	A	76	10.685	-4.656	7.240	1.00 56.27
15	483	0	ASN	Α	76	9.636	-4.897	6.642	1.00 55.41
	484	N	TRP	A	77	11.882	-4.763	6.666	1.00 53.67
	485	CA	TRP	A	77	12.007	-5.160	5.266	1.00 51.94
	486	СВ	TRP	A	77	13.469	-5.096	4.805	1.00 48.90
	487	CG	TRP	A	77	14.125	-3.744	4.934	1.00 51.60
20	488	CD2	TRP	A	77	14.156	-2.698	3.948	1.00 51.70
	489	CE2	TRP	A	77	14.900	-1.627	4.497	1.00 52.11
	490	CE3	TRP	A	77	13.628	-2.561	2.655	1.00 43.86
	491	CD1	TRP	A	77	14.826	-3.274	6.007	1.00 52.12
	492	NE1	TRP	A	77	15.295	-2.005	5.752	1.00 53.74
25	493	CZ2	TRP	Α	77	15.130	-0.436	3.799	1.00 43.91
	494	CZ3	TRP	Α	77	13.859	-1.369	1.960	1.00 37.41
	495	CH2	TRP	A	77	14.605	-0.326	2.537	1.00 35.61
	496	С	TRP	A	77	11.466	-6.574	5.063	1.00 50.29
	497	0	TRP	A	77	11.212	-7.006	3.935	1.00 54.30
30	498	N	THR	A	78	11.286	-7.280	6.172	1.00 46.30
	499	CA	THR	A	78	10.778	-8.646	6.171	1.00 40.87
	500	CB	THR	A	78	10.756	-9.200	7.602	1.00 40.94
	501	OG1	THR	A	78	12.097	-9.255	8.103	1.00 41.23
	502	CG2	THR	A	78	10.125	-10.585	7.642	1.00 43.72
35	503	С	THR	A	78	9.370	-8.747	5.597	1.00 39.63
	504	0	THR	A	78	8.927	-9.828	5.208	1.00 43.77
	505	N	ARG	A	79	8.671	-7.616	5.540	1.00.33.93
	506	CA	ARG	A	79	7.294	-7.568	5.044	1.00 29.09
	507	CB	ARG	Α	79	6.661	-6.236	5.455	1.00 22.71
40	508	CG	ARG	A	79	6.579	-6.105	6.955	1.00 24.31
	509	CD	ARG	A	79	6.030	-4.783	7.396	1.00 23.41
	510	NE	ARG	A	79	5.578	-4.870	8.778	1.00 19.61
	511	CZ	ARG	A	79	4.964	-3.891	9.431	1.00 25.88

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	555	0	VAL	A 84	l	7.455	0.240	0.895	1.00	34.73
	556	N	LYS	A 85	5	6.914	-1.471	-0.471	1.00	33.74
	557	CA	LYS	A 85	,	6.804	-0.646	-1.669	.1.00	35.59
	558	СВ	LYS	A 85	5	6.140	-1.478	-2.783	1.00	48.55
5	559	CG	LYS '	A 85	,	5.367	-0.707	-3.855	1.00	59.03
	560	CD	LYS	A 85	, ·	6.264	-0.085	-4.912	1.00	67.33
	561	CE	LYS	A 85	,	5.426	0.664	-5.948	1.00	72.93
	562	NZ	LYS	A 85	,	6.266	1.391	-6.950	1.00	68.29
	563	С	LYS	A 85	i	5.956	0.576	-1.290	1.00	33.73
10	564	0	LYS	A 85	, ,	6.393	1.716	-1.434	1.00	32.87
	565	N	PHE	A 86	;	4.760	0.305	-0.771	1.00	34.91
	566	CA	PHE	A 86		3.796	1.318	-0.334	1.00	38.00
	567	СВ	PHE	A 86	i	2.579	0.617	0.286	1.00	29.90
	568	CG	PHE .	A 86		1.520	1.553	0.814	1.00	28.19
15	569	CD1	PHE	A 86		0.306	1.694	0.150	1.00	28.34
	570	CD2	PHE,	A 86		1.703	2.237	2.014	1.00	30.14
	571	CE1	PHE .	A 86		-0.714	2.495	0.678	1.00	16.92
	572	CE2	PHE .	A 86		0.692	3.039	2.547	1.00	31.79
	573	CZ	PHE 2	A 86		-0.519	3.166	1.879	1.00	23.42
20	574	С	PHE 2	A 86		4.372	2.317	0.671	1.00	41.33
	575	0	PHE 2	A 86		4.384	3.522	0.413	1.00	44.39
	576	N	ILE Z	A 87		4.828	1.817	1.820	1.00	42.94
	5 77	ÇA	ILĘ Ż	A 87		, ,5,.390,	. 2.670	2.870	, 1.00	44.91
	578	CB	ILE A	A 87		5.999	1.842	4.021	1.00	33.27
25	579	CG2	ILE A	A 87		6.499	2.760	5.114	. 1.00	35.47
	580	CG1	ILE, 2	A 87		4.951	0.912	4.614	1.00	33.55
	581	CD1	ILE A	A 87		5.500	0.015	5.692	1.00	34.35
	582	С	ILE A	A 87		6.485	3.585	2.341	1.00	49.45
	583	0	ILE A	A 87		6.391	4.805	2.460	1.00	51.81
30	584	N	MET A	88		7.519	2.990	1.756	1.00	49.47
	585	CA	MET A	88		8.635	3.762	1.226	1.00	49.30
	586	CB	MET F	88		9.641	2.842	0.525	1.00	50.22
	587	CG	MET A	88		10.269	1.771	1.418	1.00	45.64
	588	SD	MET P	88		11.035	2.374	2.938	1.00	36.68
35	589	CE	MET F	88		12.225	3.505	2.300	1.00	32.68
	590	С	MET A	88		8.226	4.897	0.281	1.00	47.36
,	591	0	MET A	88		9.031	5.777	-0.022	1.00	47.71
	592	N	ASN A	89		6.988	4.898	-0.194	1.00	47.87
	593	CA	ASN A	89		6.582	5.981	-1.074	1.00	53.55
40	594	CB	ASN A	89		5.710	5.476	-2.219	1.00	59.69
	595	CG	ASN A	89		5.490	6.540	-3.274	1.00	60.29
	596		ASN A			6.432	6.962	-3.949	1.00	58.66
	597	ND2	ASN A	89		4.249	6.994	-3.411	1.00	59.82

		598	С	ASN	A	89	5.828	7.053	-0.300	1.00 54.69
		599	0	ASN	A	89	5.351	8.034	-0.875	1.00 55.77
		600	N	LEU	A	90	5.718	6.851	1.010	1.00 53.91
		601	CA	LEU	A	90	5.039	7.803	1.877	1.00 50.26
	5	602	СВ	LEU	A	90	4.694	7.152	3.218	1.00 44.32
		603	CG	LEU	A	90	3.552	6.134	3.213	1.00 38.54
		604	CD1	LEU	A	90	3.422	5.504	4.582	1.00 43.04
		605	CD2	LEU	A	90	2.258	6.821	2.830	1.00 42.59
		606	С	LEU	A	90	5.909	9.039	2.091	1.00 47.14
	10	607	0	LEU	A	90	5.391	10.136	2.305	1.00 44.55
		608	N	PRO	A	91	7.247	8.875	2.061	1.00 46.27
		609	CD	PRO	A	91	7.996	7.616	2.220	1.00 44.80
		610	CA	PRO	A	91	8.140	10.024	2.247	1.00 46.47
		611	СВ	PRO	A	91	9.521	9.376	2.300	1.00 43.34
	15	612	CG	PRO	A	91	9.234	8.073	2.951	1.00 45.54
		613	С	PRO	Α	91	8.009	11.030	1.094	1.00 47.41
		614	0	PRO	Α	91	8.412	12.186	1.208	1.00 46.38
		615	N	VAL	A	92	7.442	10.578	-0.020	1.00 47.94
		616	CA	VAL	A	92 .	7.249	11.439	-1.180	1.00 45.52
	20	617	CB	VAL	A	92	7.204	10.622	-2.467	1.00 34.17
		618	CG1	VAL	A	92	7.081	11.547	-3.642	1.00 38.02
		619	CG2	VAL	A	92	8.456	9.775	-2.583	1.00 38.64
		620	С	VAL	A	92	5.940	12.205	-1.026	1.00 45.50
٠		621	0	VAL	A	92	5.919	13.431	-1.117	1.00 44.68
	25	622	N	GLU	A	93	4.851	11.476	-0.791	1.00 42.90
		623	CA	GLU	A	93	3.557	12.103	-0.582	1.00 42.53
		624	CB	GLU	A	93	2.522	11.082	-0.124	1.00 49.87
		625	CG	GLU	A	93	2.449	9.818	-0.951	1.00 57.60
		626	CD	GLU	Α	93	1.189	9.021	-0.657	1.00 61.78
	30	627	OE1	GLU	A	93	1.046	7.896	-1.187	1.00 71.50
		628	OE2	GLU	A	93	0.337	9.531	0.105	1.00 52.19
		629	С	GLU	A	93	3.753	13.110	0.539	1.00 43.12
		630	0	GLU	A	93	3.322	14.255	0.452	1.00 45.85
		631	N	PHE	A	94	4.414	12.664	1.601	1.00 45.41
	35	632	CA	PHE	Α	94	4.678	13.514	2.752	1.00 46.26
		633	CB	PHE	A	94	5.575	12.787	3.756	1.00 42.53
		634	CG	PHE	A	94	5.711	13.507	5.067	1.00 32.85
		635	CD1	PHE	A	94	4.633	13.568	5.956	1.00 28.47
	-	636	CD2	PHE	A	94	6.894	14.167	5.396	1.00 28.12
	40	637	CE1			94	4.726	14.279	7.153	1.00 19.92
		638	CE2	PHE	A	94	6.999	14.882	6.590	1.00 31.07
		639	CZ	PHE	A	94	5.909	14.936	7.468	1.00 25.79
		640	С	PHE	A	94	5.346	14.817	2.326	1.00 45.67

	641	0	PHE	Δ	94	4.858	15.901	2.636	1.00 41.22
	642	N	TYR		95	6.462	14.706	1.613	1.00 44.67
	643	CA	TYR		95	7.185	15.884	1.154	1.00 42.71
•	644	СВ	TYR		95	8.467	15.487	0.430	1.00 44.48
5	645	CG	TYR		95	9.245	16.675	-0.099	1.00 45.34
	646	CD1			95	9.725	17.655	0.764	1.00 46.34
	647		TYR		95	10.449	18.740	0.292	1.00 50.00
	648	CD2	TYR	A	95	9.509	16.814	-1.458	1.00 46.57
	649	CE2	TYR	Α	95	10.230	17.895	-1.938	1.00 49.96
10	650	CZ	TYR	A	95	10.700	18.853	-1.058	1.00 53.17
	651	ОН	TYR	A	95	11.434	19.918	-1.521	1.00 55.77
	652	С	TYR	Α	95	6.352	16.738	0.215	1.00 41.47
	653	0	TYR	A	95	6.237	17.951	0.399	1.00 41.86
	654	N	ASP	A	96	5.782	16.105	-0.804	1.00 38.09
15	655	CA	ASP	A	96	4.975	16.838	-1.761	1.00 34.86
	656	CB	ASP	A	96	4.278	15.907	-2.751	1.00 28.63
•	657	CG	ASP	A	96	5.178	15.499	-3.898	1.00 32.06
	658	OD1	ASP	A	96	6.190	16.203	-4.142	1.00 29.64
	659	OD2	ASP	A	96	4.857	14.482	-4.561	1.00 33.25
20	660	С	ASP	A	96	3.924	17.694	-1.100	1.00 31.39
	661	0	ASP	A	96	3.933	18.908	-1.268	1.00 31.77
	662	N	ASN	A	97	3.025	17.087	-0.335	1.00 26.14
	663	CA	ASN	A	97.	1.976	17.889	0.269	1.00 29.32.
	664	CB	ASN	A	97	0.650	17.565	-0.433	1.00 34.58
25	665	CG	ASN	A	97	0.375	16.077	-0.515	1.00 33.64
	666	OD1	ASN	A	97	-0.464	15.628	-1.310	1.00 31.70
	667		ASN		97	1.067	15.299	0.319	1.00 25.32
	668	С	ASN		97	1.790	17.924	1.791	1.00 33.75
20	669	0	ASN		97	0.826	18.521	2.275	1.00 31.16
30	670	N	TYR		98	2.699	17.319	2.552	1.00 37.18
	671	CA	TYR		••	2.586	17.361	4.012	
	672	СВ	TYR		98	2.683	15.966	4.605	1.00 33.51
	673	CG	TYR		98	1.360	15.282	4.649	1.00 29.03
25	674		TYR		98.	0.990	14.378	3.656	1.00 24.71
35	675		TYR		98	-0.266	13.797	3.651	1.00 19.15
	676		TYR		98	0.445	15.589	5.645	1.00 24.62
	677		TYR		98	-0.814	15.022	5.655	1.00 22.79
	678.	CZ	TYR		98	-1.168	14.125	4.652	1.00 25.75
40	679	ОН	TYR		98	-2.433	13.574	4.644	1.00 31.99
40	680		TYR		98	3.645		4.649	1.00 36.88
	681		TYR		98	3.412	18.883	5.691	1.00 38.14
	682		VAL		99	4.811	18.293	4.012	1.00 34.30
•	683	CA	VAL	A	99	5.932	19.105	4.465	1.00 27.39

	60.4	-		_	0.0		7 102		3.658	1 00	20.34
	684 685	CB CG1	VAL		99 99		7.193 8.284	18.760 19.772			16.92
			VAL		99		7.661		4.021		19.75
	686						5.646	20.614			31.44
5	687	C	VAL		99			21.371			35.10
5	688	0	VAL				6.009				34.59
	689	N			100	•	4.991	21.072			
	690	CD			100		4.444				35.82
	691	CA			100		4.706				33.54
4.0	692	CB			100	'	3.679				31.42
10	693	CG			100		4.144				35.80
	694	С	•		100		4.147				34.59
	695	0			100		4.646		,5.027		36.94
	696	N	GLU	A	101		3.117				33.67
•	697	CA	GLU	A	101		2.481	22.785			,31.97
15	698	CB			101	•	1.248	21.937			16.92
	699	CG	GLU	A	101		0.725	22.160	7.935	1.00	16.92
	700	CD	GĽÚ	A	101		-0.679	21.648	8.139	1.00	26.55
•	701	OE1	GLU	Α	101		-0.967	20.504	7.711	1.00	21.07
	702	OE2	GLU	A	101		-1.484	22.396	8.743	1.00	22.12
20	703	С	GLU	A	101	•	3.394	22.744	7.459	1.00	33.18
	704	0	GLU	A	101		3.421	23.682	8.258	1.00	32.52
	705	N	LEU	A	102		4.121	21.648	7.624	1.00	33.81
	706	CA	LEU	Α,	102		5.019	21.560	8.756	1.00	31.47
	707	CB	LEÜ	À	102	2000	5.820	20.262	8.694	1.00	30.43
25	708	CG	LEU	A	102		4.974	18.997	8.837	1.00	34.74
	709	CD1	LEU	Α	102	1	5.866	17.776	8.764	1.00	25.10
	710	CD2	LEU	Α	102		4.232	19.029	10.162	1.00	36.87
	711	С	LEU	A	102		5.942	22.769	8.685	1.00	30.29
	712	0	LEU	Α	102		6.206	23.429	9.694	1.00	33.60
30	713	N	HIS	A	103		6.398	23.067	7.471	1.00	28.12
	714	CA	HIS	A	103		7.298	24.186	7.214	1.00	30.58
	715	СВ	HIS	A	103		7.735	24.153	5.760	1.00	32.00
	716	CG	HIS	Α	103		8.864	25.083	5.451	1.00	35.36
	717	CD2	HIS	Α	103		8.953	26.123	4.590	1.00	34.89
35	718	ND1	HIS	A	103		10.104	24.967	6.042	1.00	38.53
	719	CE1	HIS	Α	103		10.909	25.894			36.15
	720		HIS				10.235	26.608			34.36
	721	С	HIS				6.677				31.60
	722	0	HIS				7.365				26.65
40	723	N			104		5.378	25.672			30.94
-	724	CA			104		4.694				28.23
	725	СВ			104		3.284		7.056		
	726	С	ALA				4.677		· ·		32.92
	, 20	J	unu	~	T 0 4		3.077	21.000	9.U3I	1.00	24.96

	727	0	ALA	À	104	4.762	28.128	9.631	1.00	40.90
	728	N	ASN	Α	105	4.580	25.897	9.773	1.00	32.79
	729	CA	ASN	Α	105	4.543	25.899	11.233	1.00	29.90
	730	СВ	ASN	A	105	3.645	24.762	11.739	1.00	42.45
5	.731	CG	ASN	·A	105	2.169	25.048	11.509	1.00	48.96
	732	OD1	ASN	Α	105	1.617	25.989	12.076	1.00	60.59
	733	ND2	ASN	A	105	1.529	24.245	10.667	1.00	37.91
	. 734	С	ASN	Α	105	5.915	25.846	11,909	1.00	24.31
	735	0	ASN	A	105	6.030	25.474	13.075	1.00	24.21
10	736	N	ASN	Ą	106	6.950	26.228	11.167	1,00	21.42
	737	CA	ASN	A	106	8.314	26.278	11.687	1.00	21.95
	738	CB	ASN	Α	106	8.390	27.294	12.834	1.00	16.92
	739	ÇG	ASN	A	106	9.818	27.682	13.180	1.00	18.90
	740	OD1	ASN	A	106	10.091	28.173	14.275	1.00	20.83
15	741	ND2	ASN	. A	106	10.736	27.473	12.238	1.00	16.92
	742	С	ASŅ	A	106	8.854	24.937	12.177	1.00	26.82
	743	0	ASN	A	106	9.655	24.892	13.111	1.00	28.64
	744	N	VAL	A	107	8.430	23.842	11.561	1:00	28.06
	745	CA	VAL	A	107	8.914	22.538	11.988	1.00	25.22
20	746	CB	VAL	A	107	7.825	21.456	11.791	1.00	24.13
	747	CG1	VAL	A	107	8.322	20.100	12.286	1.00	37.12
	748	CG2	VAL	A	107	6.560	21.865	12.528	1.00	24.46
	.749	C	VΆĻ	A'	107	10.152	22.172	11.176	1.00	28.07
	750	0			107			9.962	1.00	33.25
25	751	N	LYŚ	A	108 · ·	11.199	21.698	11.847	1.00	25.06
	752	CA	LYS	·A	108	12.422	21.280	11.157	1.00	24.60
	753	CB				13.665	21.628	11.975	1.00	19.20
	754	CG			108	14.972		11.350	1.00	17.42
	755	CD			108	16.158	21.849	12.020	1.00	18.52
30	756	CE			108	17.488	21.171	11.715	1.00	23.17
	757	NZ			108			10.267		
	758	С			108	12.325	19.771	10.976		28.32
	759	0			108	11.738		11.808		32.57
0.5	760	N			109	12.882				29.02
35	761	CA			109	12.797				29.85
	762	CB			109	11.940	17.492			29.54
	763	CG2				11.773				24.76
	764	CG1				10.557	18.139			26.25
40	765	CD1				9.602	17.740			26.43
40	766	C			109	14.171	17.176			31.25
	767		ILE			15.019	17.653			31.58
	768		GLN			14.383		10.283		34.94
	769	CA	GLN	A	110	15.636	15.360	10.254	1.00	35.94

	770	СВ	GLN	Α	110	16.491	15.699	11.472	1.00 43.90
	771	CG	GLN	A	110	16.579	17.182	11.769	1.00 52.49
	772	CD	GLN	Α	110	17.578	17.513	12.860	1.00 53.12
	773	OE1	GLN	Α	110	17.710	18.673	13.266	1.00 42.83
5	774	NE2	GLN	A	110	18.298	16.496	13.338	1.00 66.31
	775	C ;	GLN	Α	110	15.264	13.892	10.293	1.00 35.02
	776	0	GLN	Α	110	14.195	13.534	10.792	1.00 36.09
	777	N	MET	A	111	16.135	13.044	9.762	1.00 34.95
	778	CA	MET	A	111	15.879	11.613	9.758	1.00 38.29
10	779	CB	MET	A	111	15.299	11.184	8.401	1.00 54.75
•	780	CG	MET	A	111	16.107	11.572	7.159	1.00 63.44
	781	SD	MET	Α	111	17.262	10.296	6.580	1.00 75.55
	782	CE	MET	A	111	16.222	8.800	6.651	1.00 63.96
	783	С	MET	A	111	17.137	10.816	10.093	1.00 39.52
15	784	0	MET	Α	111	18.190	11.030	9.501	1.00 42.08
	785	N	İLE	A	112	17.018	9.903	11.057	1.00 39.74
	786	CA	ILE	A	112	18.140	9.069	11.494	1.00 38.26
	787	СВ	ILE	A	112	18.291	9.077	13.030	1.00 37.80
	788	CG2	ILE	A	112	18.536	10.490	13.526	1.00 34.53
20	789	CG1	ILE	A	112	17.039	8.470	13.667	1.00 42.15
•	790	CD1	ILE	A	112	17.143	8.260	15.149	1.00 40.41
	791	С	ILE	A	112	17.978	7.612	11.078	1.00 33.52
	792	0	ILE	A	112	16.862	7.104	10.969	1.00 28.71
1	793	N	GLY	A	113	19.104	6.943	10.860	1.00 30.89
25	794	CA	GLY	A	113	19.061	5.547	10.485	1.00 37.18
	795	С	GLY	A	113	19.963	5.229	9.322	1.00 39.38
	796	0	GLY	A	113	20.621	6.113	8.785	1.00 38.55
	797	N	GLU	A	114	19.994	3.954	8.944	1.00 42.25
	798	CA	GLU	A	114	20.802	3.489	7.826	1.00 50.83
30	799	CB	GLU	A	114	20.946	1.961	7.878	1.00 64.49
	800	CG	GLU	A	114	21.957	1.446	8.913	1.00 73.99
	801	CD	GLU	A	114	21.327	0.579	9.988	1.00 75.69
	802	OE1	GLU	A	114	20.709	1.131	10.927	1.00 75.15
	803	OE2	GLU	A	114	21.449	-0.661	9.888	1.00 71.34
35	804	С	GLU	A	114	20.102	3.923	6.542	1.00 55.84
	805	0	GLU	A	114	19.401	3.148	5.895	1.00 57.72
	806	N	THR	A	115	20.311	5.183	6.189	1.00 57.14
	807	CA	THR	A	115	19.697	5.786	5.017	1.00 58.68
	808	CB				19.866	7.297	5.065	1.00 53.84
40	809	OG1	THR	A	115	21.235	7.618	4.805	1.00 53.59
	810	CG2			115	19.488	7.830	6.443	1.00 49.34
	811	С	THR	A	115	20.256		3.684	1.00 63.08
	812	0	THR	A	115	19.840	5.791	2.635	1.00 63.55

	813	N	ASP A	116	21.186	4.363	3.713	1.00	67.68
	814	CA	ASP A	116	21.799	3.880	2.480	1.00	72.55
	815	СВ	ASP A	116	23.270	3.539	2.737	. 1.00	76.81
	816	CG	ASP A	116	24.099	4.767	3.082	1.00	82.99
5	817	OD:	L ASP A	116	23.821	5.405	4.121	1.00	84,93
	818	OD2	2 ASP A	116	25.025	5.098	2.310	1.00	75.26
	819	С	ASP A	116	21.117	2.713	1.772	1.00	74.26
	820	0	ASP A	116	21.426	2.430	0.614	1.00	76.40
	821	N	ARG A	117	20.196	2.034	2.448	1.00	75.22
10	822	CA	ARG A	117	19.494		1.828	1.00	76.00
	823	CB	ARG A	117	19.350	-0.249	2.824	1.00	91.55
	824	CG	ARG A	117	20.511	-0.377	3.803	1.00	106.10
	825	CD	ARG A				4.725	1.00	116.76
	826		ARG A				5.992		125.02
15	827	CZ	ARG. A			-1.107			129.50
	828		•						133.15
	829			117		•	7.300		
	830	С		117					73.15
20	831	0		117	17.267		0.952		75.52
20	832	N	LEU A				1.472		65.43
	833	CA			16.622				
	834	СВ			16.446				53.32
	835		•		16.371				
25	836			118			3.814		
23	837				15.189	•	•		
	838 839	с 0	•	118	16.463		-0.382		
	840	N			17.432 15.220				56.56
	841	CD	PRO A		14.050		-0.863		47.23
30	842	CA	PRO A	•	14.030	3.750	-0.157 -2.272		48.03
	843	СВ	PRO A		13.411		-2.330		44.88
	844	CG	PRO A		13.193		-1.286		43.34
	845	С	PRO A		15.305		-2.577		50.30
	846	0	PRO A		15.220		-1.706		51.90
35	847	N	LYS A		15.722		-3.805		52.17
	848	CA	LYS A		16.137		-4.166		56.36
	849	СВ	LYS A		16.618		-5.617		63.53
	850	CG	LYS A		17.297		-6.000		63.00
	851	CD	LYS A		17.350		-7.509		73.77
40	852	CE	LYS A		15.955		-8.070		77.05
	853	NZ	LYS A		15.992		-9.510		69.29
	854	С	LYS A		15.056				55.74
	855	0	LYS A		15.253		-3.258		56.30
					-,				

	856	N	GLN	A	121		13.920	7.704	-4.649	1.00	55.41
	857	CA	GLN	A	121		12.840	8.675	-4.559	1.00	54.91
	858	СВ	GLN	A	121		11.614	8.206	-5.359	1.00	67.90
	859	CG	GLN	Α	121		10.674	7.252	-4.630	1.00	74.11
5	860	CD	GLN	Α	121		11.197	5:837	-4.544	1.00	76.82
	861	OE1	GLN	Α	121		10.562	4.967	-3.945	1.00	72.18
	862	NE2	GLN	A	121		12.355	5.593	-5.147	1.00	76.38
	863	С	GLN	Α	121		12.466	8.916	-3.104	1.00	52.21
	864	0	GLN	A	121		12.071	10.018	-2.728	1.00	53.09
10	865	N	THR	A	122		12.604	7.878	-2.286	1.00	49.30
	866	CA	THR	A	122		12.290	7.973	-0.862	1.00	43.48
	867	СВ	THR	A	122		12.344	6.585	-0.179	1.00	42.07
	868	OG1	THR	A	122		11.548	5.650	-0.918	1.00	47.12
	869	CG2	THR	A	122		11.827	6.677	1.251	1.00	43.57
15	870	С	THR	A	122		13.329	8.865	-0.189	1.00	35.33
	871	0	THR	Α	122		13.001	9.836	0.504	1.00	27.53
	872	N	PHE	A	123		14.590	8.512	-0.406	1.00	33.58
	873	CA	PHE	A	123		15.706	9.239	0.166	1.00	35.10
	874	СВ	PHE	A	123 -		17.022	8.656	-0.330	1.00	37.63
20	875	CG	PHE	A	123		18.222	9.257	0.318	1.00	44.54
	876	CD1	PHE	Α	123		18.427	9.116	1.688	1.00	53.52
	877	CD2	PHE	A	123		19.145	9.972	-0.432	1.00	46.30
	878	CE1	PHE	A	123		19.539	9.679	2.304	1.00	61.21
,	879	CE2	PHE	A	123	•	20.262	10.541	0.173	1.00	47.50
25	880	CZ	PHE	A	123		20.459	10.394	1.544	1.00	55.61
•	881	С	PHE	Α	123		15.632	10.698	-0.223	1.00	37.43
	882	0	PHE	A	123		15.521	11.575	0.636	1.00	39.83
	883	N	GLU	A	124		15.693	10.950	-1.525	1.00	37.07
	884	CA	GLU	A	124		15.637	12.305	-2.038	1.00	35.49
30	885	CB	GLU	A	124		15.495	12.274	-3.552	1.00	33.74
	886	CG	GLU	A	124		16.775	11.871	-4.251	1.00	34.11
	887	CD	GLU	A	124		16.563	11.549	-5.712	1.00	43.15
	888	OE1	GLU	A	124		17.570	11.327	-6.420	1.00	48.58
	889	OE2	GLU	Α	124		15.390	11.511	-6.150	1.00	60.13
35	890	С	GLU	Α	124		14.499	13.096	-1.419	1.00	35.66
	891	0	GLU	A	124		14.661	14.274	-1.112	1.00	36.51
	892	N	ALA	A	125		13.356	12.450	-1.219	1.00	34.75
	893	CA	ALA	A	125		12.207	13.124	-0.629	1.00	37.21
•	894	CB	ALA	Α	125		11.065	12.146	-0.453	1.00	34.20
40	895	С	ALA	A	125		12.576	13.730	0.715	1.00	40.90
	896	0	ALA	A	125		12.393	14.926	0.946	1.00	44.51
	897	N	LEU	A	126		13.104	12.894	1.598	1.00	39.91
	898	CA	LEU	A	126		13.490	13.331	2.929	1.00	38.45

	899	CB	LEU	A 126		13.847	12.114	3.773	1.0	0 36.01
	900	CG	LEU	A 126		12.648	11.198	4.027	1.0	28.88
	901	CD	1 LEU	A 126		13.135	9.787	4.318	1.00	32.10
	902	CD	2 LEU	A 126		11.803	11.764	5.167	1.00	22.64
5	903	С	LEU	A 126		14.650	14.306	2.900	1.00	39.09
	904	0.	LEU	A 126		14.644	15.313	3.595	1.00	41.65
	905	N	THR	A 127		15.652	13.998	2.097	1.00	36.98
	906	CA	THR	A 127		16.810	14.864	1.971	1.00	42.37
	907	СВ	THR	A 127		17.677	14.406	0.801	1.00	49.56
. 10	908	OG	1 THR	A 127		18.086	13.050	1.023	1.00	47.49
	909	CG.	2 THR	A 127		18.893	15.294	0.657	1.00	48.08
	910	С	THR .	A 127		16.352	16.299	1.726	1.00	46.79
	911	0	THR .	A 127	•	16.787	17.232	2.405	1.00	50.37
	912	N	LYS .	A 128		15.463	16.456	0.749	1.00	49.56
15	913.	CA	LYS 2	A 128		14.914	17.754	0.387	1.00	46.71
	914	CB	LYS I	A 128		14.019	17.616	-0.848	1.00	47.68
	915	CG	LYS A	A 128		14.777	17.671	-2.171	1.00	55.98
	916	CD	LYS 2	A 128		14.193	16.722	-3.211	1.00	60.97
	917	CE	LYS A	A 128		12.713	16.978	-3.451	1.00	65.54
20	918	NZ	LYS A	A 128		12.070	15.978	-4.364	1.00	64.13
	919	С	LYS A	A 128		14.126	18.376	1.531	1.00	45.28
	920	0	LYS A	A 128		14.382	19.513	1.918	1.00	41.48
	921	N		A 129		13.168	17.635	2.073	1.00	45.11
	922	CA	ALA A			12.359	18.145	3.177	1.00	46.45
25.	923	CB	ALA A			11.411	17.068	3.665	1.00	49.46
	924	С	ALA A	129		13.229	18.634	4.332	1.00	44.27
	925	0	ALA A	129		12.800	19.463	5.132	1.00	41.06
	926	N	GLU A			14.445	18.099	4.418	1.00	44.20
20	927	CA	GLU A			15.391	18.487	5.455	1.00	46.78
30	928	CB	GLU A			16.494	17.442	5.599	1.00	44.22
	929	CG		130	•		16.064	6.000	1.00	49.59
	930	CD	GLU A			17.142	15.111	6.324	1.00	49.64
	931		GLU A			17.967	14.821	5.427	1.00	49.46
25	932		GLU A			17.209	14.652	7.484		53.99
35	933	С	GLU A			16.004	19.782	4.989	1.00	48.99
	934	0	GLU A			16.207	20.715	5.764	1.00	48.82
	935	N	GLU A			16.300	19.810	3.697	1.00	47.76
	936	CA		131		16.879	20.969	3.046	1.00	41.07
40	937	СВ	GLU A			17.122	20.653	1.573	1.00	33.82
40	938	CG	GLU A			18.573	20.638	1.213		48.83
	939	CD	GLU A			19.281	21.865	1.754		53.69
	940		GLU A			18.859				54.79
	941	OE2	GLU A	131		20.251	21.699	2.529	1.00	67.98

	942	C.	GLU A	131	15.954	22.179	3.170	1.00	39.85
	943	0	GLU A	131	16.388	23.289	3.481	1.00	39.50
	944	N	LEU A	132	14.671	. 21.957	2.926	1.00	40.81
	945	CA	LEU A	132	13.686	23.023	3.008	1.00	40.93
5	946	СВ	LEU A	132	12.303	22.480	2.631	1.00	42.02
	947	CG	LEU' F	132	11.104	23.429	2.735	1.00	37.20
	948	CD:	1 LEU P	132	11.372	24.670	1.914	1.00	40.73
	949	CD:	2 LEU A	132	9.840	22.736	2.246	1.00	22.65
	950	С	LEU A	132	13.630	23.631	4.401	1.00	39.99
10	951	0	LEU A	132	13.697	24.845	4.565	1.00	37.40
	952	N	THR A	133	13.533	22.767	5.404	1.00	43.53
	953	CA	THR A	133	13.416	23.187	6.797	1.00	43.29
	954	СВ	THR A	133	12.535	22.179	7.565	1.00	30.42
	955	OG I	L THR A	133	12.944	20.842	7.242	1.00	32.09
15	956	CG2	THR A	133	11.076	22.353	7.178	1.00	29.55
	957	С	THR A	. 133	14.686	23.450	7 [.] .618	1.00	40.62
	958	0	THR A	. 133	14.588	23.716	8.817	1.00	37.19
	959	Ń	LYS A	134	15.858	23.393	6.985	1.00	34.90
	960	CA	LYS A	134	17.126	23.639	7.683	1.00	36.42
20	961	CB	LYS A	134	18.223	24.079	6.713	1.00	20.34
	962	CG	LYS A	134	18.756	23.011	5.786	1.00	39.12
	963	CD	LYS A	134	19.867	23.565	4.875	1.00	44.98
	964	CE	LYS A	134	19.364	24.690	3.969	1.00	44.22
	965	NZ	LYS A	134	20.388	25.145	2.986	1.00	45.46
25	966	С	LYS A	134	17.033	24.715	8.751	1.00	44.36
	967	0	LYS A	134	17.078	24.432	9.945	1.00	48.76
	968	N			16.905	25.958	8.303	1.00	49.25
	969	CA	ASN A	135	16.853	27.099	9.202	1.00	49.89
	970	CB	ASN A	135	17.041	28.398	8.413	1.00	51.24
30	971	CG	ASN A			28.291			
	972				19.136	27.616	7.555	1.00	47.82
	973	ND2	ASN A		17.923	28.970	6.237	1.00	67.17
	974	С	ASN A		15.610	27.229	10.072	1.00	51.52
25	975	0	ASN A	135	15.421	28.261	10.715	1.00	52.67
35	976	N	ASN A		14.754	26.213	10.099	1.00	51.08
	977	CA			13.567	26.307	10.942	1.00	50.58
	978	CB	ASN A		12.529	25.261	10.544	1.00	44.34
	979	CG	ASN A		11.579	25.769	9.477	1.00	37.46
40	980		ASN A		10.561	25.144		1.00	26.38
40	981		ASN A		11.907	26.910	8.880	1.00	42.23
-	982	С	ASN A		13.949	26.157	12.410	1.00	51.60
	983	0	ASN A		14.959		12.739		53.87
	984	N	THR A	137	13.142	26.724	13.297	1.00	50.58

	985	CA	THR A 137		13.458	26.671	14.711	1.00 46.19
	986	CB	THR A 137		13.846	28.054	15.207	1.00 44.64
	987	OG:	1 THR A 137		12.770	28.959	14.951	1.00 35.45
	988	CG2	2 THR'A 137		15.082	28.542	14.499	1.00 28.58
5	989	С	THR A 137		12.347	26.155	15.610	1.00 44.33
	990	0	THR A 137	•	12.276	26.531	16.784	1.00 47.55
	991	N	GLY A 138	. •	11.479	25.303	15.080	1.00 40.76
	992	CA	GLY A 138		10.400	24.775	15.899	1.00 38.50
	993	С	GLY A 138		10.707	23.363	16.349	1.00 37.87
10	994	0	GLY A 138.		11.874	22.969	16.433	1.00 35.95
	995	N	LEU A 139		9.662	22.602	16.649	1.00 37.09
	996	CA	LEU A 139		9.832	21.214	17.063	1.00 37.28
	997	CB	LEU A 139		8.460	20.535	17.193	1.00 41.93
	998	CG	LEU A 139		8.337	19.053	17.575	1.00 43.42
15	999	CD1	LEU A 139		6.873	18.749	17833	1.00 36:62
	1000	CD	2 LEU A 139		8.880	18.145	16.480	1.00 40.37
	1001	С	LEU A 139		10.635	20.544	15.959	1.00 35.36
	1002	0	LEU A 139		10.531	20.940	14.798	1.00 34.33
	1003	N	ILE A 140		11.440	19.548	16.306	1.00 33.22
20	1004	CA	ILE A 140	•	12.207	18.854	15.286	1.00 32.63
	1005	CB	ILE A 140		13.655	18.645	15.699	1.00 23.68
	1006	CG:	2 ILE A 140		14.432	18.033	14.548	1.00 18.34
	1007	CG:	4.0		14.269	19.975	16.108	1.00 19.23
	1008	CD:	1 ILE A 140		15.655	19.844	16.651	1.00 16.92
25	1009	С	ILE A 140	٠٠.	11.578	17.496	15.065	1.00 -33.01
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	1011	N	LEU A 141		11.021	17.290	13.879	1.00 29.19
	1012	CA	LEU A 141		10.397	16.017	13.566	1.00 27.02
20	1013	СВ	LEU A 141		9.327	16.205	12.499	1.00 16.92
30	1014	CG	LEU A 141		8.207	15.173		1.00 17.32
	1015		LEU A 141			15.618	11.662	1.00 16.92
	1016				8.748	13.827	12.129	1.00 16.92
	1017	С	LEU A 141		11.495	15.076	13.087	1.00 28.94
25	1018	0				15.103	11.927	1.00 25.64
35	1019	N	ASN A 142		11.962	14.249	14.014	1.00 31.00
	1020	CA			13.032	13.309	13.753	1.00 33.31
	1021	СВ	ASN A 142		13.838	13.150	15.035	1.00 23.76
	1022	CG	ASN A 142			12.806	14.778	1.00 30.31
40	1023		ASN A 142		15.962	13.478	14.009	1.00 44.03
40	1024		ASN A 142		15.763	11.762	15.432	1.00 27.58
	1025	С	ASN A 142		12.493	11.960	13.285	1.00 38.34
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	1073	С	GLY A 14	8 18.628	0.068	15.692	1.00 36.55
	1074	0	GLY A 14	8 19.794	0.440	15.601	1.00 34.11
5	1075	N	GLY A 14	9 18.013	-0.085	16.858	1.00 35.88
	1076	CA	GLY A 14	9 18.703	0.187	18.106	1.00 35.86
	1077	С	GLY A 14	9 20.111	-0.372	18.193	1.00 33.73
	1078	0	GLY A 14	21.093	0.372	18.130	1.00 34.86
	1079	N	ARG A 15	20.221	-1.685	18.345	1.00 29.19
. 10	1080	CA	ARG A 15	21.528	-2.315	18.450	1.00 28.55
	1081	СВ	ARG A 15	21.378	3.830	18.591	1.00 21.40
	1082	CG	ARG A 150	20.591	-4.283	19.817	1.00 21.80
	1083	CD	ARG A 150	20.657	-5.792	19.979	1.00 16.92
	1084	NE	ARG A 150	19.782	-6.260	21.046	1.00 16.92
15	1085	CZ	ARG A 150	19.684	-7.531	21.433	1.00 19.59
	1086	NHI	1 ARG A 150	20.414	-8.471	20.839	1.00 23.32
	1087	NH2	2 ARG A 150	18.847	-7.872	22.409	1.00 21.38
	1088	С	ARG A 150	22.378	-1.989	17.227	1.00 30.06
	1089	.0	ARG A 150	23.603	-1.875	17.310	1.00 26.00
20	1090	N	ALA A 151	21.719	-1.838	16.088	1.00 35.94
	1091	CA	ALA A 151	22.422	-1.517	14.859	1.00 37.38
	1092	СВ	ALA A 151	21.438	-1.469	13.698	1.00 52.48
	1093	С	ALA A 151	23.156	-0.179	14.990	1.00 35.17
	1094	0	ALA A 151	24.338	-0.080	14.656	1.00 31.19
25 .	1095	N	GLU A 152	22.451	0.844	15.474	1.00 32.94
	1096	CA	GLU A 152	23.033	2.171	15.650	1.00 35.48
	1097	СВ	GLU A 152	21.992	3.143	16.207	1.00 30.00
	1098	CG	GLU A 152	22.577	4.440	16.751	1.00 19.49
	1099	CD	GLU A 152	21.535	5.292	17.460	1.00 22.76
30	1100	OE1	GLU A 152	20.658	4.718	18.145	1.00 21.18
	1101	OE2	GLU A 152	21.595	6.539	17.351	1.00 25.44
	1102	С	GLU A 152	24.241	2.148	16.576	1.00 38.76
	1103	0	GLU A 152	25.270	2.743	16.259	1.00 39.19
	1104	N	ILE A 153	24.116	1.473	17.718	1.00 39.55
35	1105	CA	ILE A 153	25.219	1.396	18.677	1.00 38.31
	1106	CB	ILE A 153	24.817	0.652	19.964	1.00 32.60
	1107	CG2	ILE A 153	25.968	0.664	20.942	1.00 35.83
	1108	CG1	ILE A 153	23.601	1.316	20.601	1.00 37.55
	1109	CD1	ILE A 153	23.133	0.639	21.862	1.00 34.30
40	1110	С	ILE A 153	26.424	0.676	18.086	1.00 40.62
	1111	0	ILE A 153	27.565	1.043	18.352	1.00 37.23
	1112	N	THR A 154	26.157	-0.353	17.286	1.00 45.36
	1113	CA	THR A 154	27.209	-1.140	16.647	1.00 47.53

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               LEU A 159
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                                              15.097
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	1157	0	LEU	J A	159	35.552	5.070	14.745	1.00	32.72
	1158	N	ILE	: <i>P</i>	160	34.180	4.346	16.372	1.00	39.18
	1159	CA	ILE	: A	160	35.110	4.661	17.451	1.00	39.26
	1160	СВ	ILE	A	160	34.451	4.464	18.828	1.00	29.65
5	1161	CG2	2 ILE	A	160	35.467	4.701	19.939	1.00	21.54
	1162	CG:	LILE	: A	160	33.274	5.424	18.981	1.00	33.17
	1163	CD:	LILE	: A	160	32.497	5.216	20.252	1.00	27.59
	1164	С	ILE	: A	160	36.346	3.768	17.358	1.00	42.75
	1165	0	ILE	A	160	37.472	4.253	17.404	1.00	41.60
. 10	1166	N	SER	A	161	36.138	2.463	17.224	1.00	47.98
	1167	CA	SER	A	161	37.261	1.539	17.113	1.00	52.98
	1168	СВ	SER	A	161	36.779	0.087	17.167	1.00	51.83
	1169	OG	SER	A	161	36.293	-0.244	18.457	1.00	47.45
	1170	С	SER	A	161	37.998	1.778	15.805	1.00	54.93
15	1171	0	SER	A	161	38.787	0.945	15.366	1.00	59.36
	1172	N	GLN	Α	162	37.722	2.915	15.177	1.00	54.75
	1173	CA	GLN	Α	162	38.367	3.277	13.927	1.00	57.55
	1174	СВ	GLN	Α	162	37.323	3.550	12.849	1.00	57.42
	1175	·CG	GLN	Α	162	37.917	3.877	11.489	1.00	59.30
20	1176	CD	GLN	A	162	38.609	2.687	10.859	1.00	61.11
	11.77	OE1	GLN	A	162	39.542	2.125	11.427	1.00	65.88
	1178	NE2	GLN	A	162	38.152	2.296	9.676	1.00	72.94
	1179	С	GLN	A	162	39.194	4.530	14.176	1.00	60.23
	1180	0	GLN	A	162	40.353	4.614	13.776	1.00	61.01
25.	1181	N	ASP	A	163	38.587	5.507	14.839	1.00	61.53
	1182	CA	ASP	A	163	39.277	6.745	15.166	1.00	59.20
	1183	CB	ASP	A	163	38.298	7.743	15.792	1.00	59.79
	1184	CG			163	37.203	8.170	14.834	1.00	63.02
	1185	OD1	ASP	A	163	36.632	7.292	14.158	1.00	72.81
30	1186	OD2	ASP	Ą	163	36.904	9.380	14.762	1.00	61.86
	1187	С			163	40.388	6.400	16.159	1.00	57.70
	1188	0	ASP	A	163	41.429		16.193	1.00	55.82
	1189	N			164	40.151	5.367	16.963	1.00	57.73
~ ~	1190	CA				41.119	4.914	17.953	1.00	59.37
35		СВ			164	40.519	3.862	18.891	1.00	55.59
	1192		VAL			41.604	3.296	19,801	1.00	47.40
	1193	CG2	VAL	A		39.416	4.479	19.714	1.00	51.18
	1194	С				42.286	4.270	17.242	1.00	62.08
4.6	1195	0			164	43.447		17.573	1.00	65.19
40	1196	И	LEU			41.963		16.268	1.00	63.92
	1197	CA	LEU			42.978		15.490	1.00	62.86
	1198	CB	LEU	A	165	42.311		14.555		45.47
	1199	CG	LEU	Α	165	43.218	0.747	13.834	1.00	40.70

	1200	CD1	LEU.	A	165		42.521	-0.595	13.698	1.00	39.99
	1201	CD2	LEU	A	165		43.592	1.318	12.485	1.00	39.90
	1202	·C	LEU	A	165		43.750	3.796	14.704	1.00	63.35
	1203	0	LEU	Α	1.65		44.981	3.788	14.683	1.00	63.16
5	1204	N	ASP	A	166		43.020	4.713	14.076	1.00	64.85
	1205	CA	ASP	A	166		43.634	. 5.793	13.312	1.00	65.80
	1206	СВ	ASP	A	166		42.581	6.521	12.477	1.00	71.82
	. 1207	CG	ASP	A	166		42.153	5.728	11.263	1.00	70.86
	1208	OD1	ASP	A	166		41.740	4.561	11.428	1.00	65.25
10	1209	OD2	ASP	Α	166		42.227	6.272	10.141	1.00	80.37
	1210	С	ASP	Α	166		44.298	6.781	14.265	1.00	66.21
	1211	0	ASP	A	166		44.567	7.927	13.903	1.00	65.89
	1212	N	ALA	A	167		44.552	6.323	15.488	1.00	66.17
	1213	CA	ALA	Α	167		45.185	7.138	16.519	1.00	66.51
15	1214	СВ	ALA	Α	167·		46.691	7.204	16.277	1.00	63.12
	1215	С	ALA	A	167		44.602	8.547	16.600	1.00	67.20
	1216	0	ALA	A	167		45.170	9.499	16,067	1.00	64.87
	1217	N	LYS	A	168		43.457	8.666	17.264	1.00	69.56
	1218	CA	LYS	A	168		42.800	9.954	17.444	1.00	70.73
20	1219	CB	LYS	A	168		41.515	10.034	16.629	1.00	55.74
	1220	CG	LYS	A	168		41.739	10.195	15.158	1.00	43.98
	1221	CD	LYS	A	168		40.450	10.600	14.486	1.00	50.77
	1222	CE	LYS	A	168		40.682	10.922	13.021	1.00	54.71
	1223	NZ	LYS	A	168	' , '	41.325	9.779	12.312	1.00	56.54
25	1224	С	LYS	Α	168		42.466	10.129	18.909	1.00	74.61
	1225	0	LYS	Α	168		42.990	11.020	19.580	1.00	79.29
	1226	N	ILE	A	169		41.583	9.272	19.401	1.00	75.01
	1227	CA	ILE	Α	169		41.196	9.325	20,795	1.00	77.20
	1228	СВ	ILE	A	169		39.651	9.321	20,960	1.00	70.32
30	1229	CG2	ILE	Α	169		39.053	10.497	20.203	1.00	64.44
	1230	CG1	ILE	A	169		39.049	8.011	20.444	1.00	67.21
	1231	CD1	ILE	A	169		39.169	7.812	18.957	1.00	62.39
	1232	С	ILE	A	169		41.805	8.112	21.478	1.00	81.65
	1233	0	ILE	A	169		41.777	7.008	20.933	1.00	82.71
35	1234	N	ASN	A	170		42.384	8.328	22.656	1.00	84.48
	1235	CA .	ASN	A	170		43.003	7.240	23.402	1.00	86.01
	1236	CB	ASN	A	170		43.440	7.699	24.803	1.00	99.20
	1237	CG	ASN	A	170		44.062	9.090	24.809	1.00	105.24
	1238	OD1	ASN	A	170		44.731	9.491	23.855	1.001	109.37
40	1239	ND2	ASN	A	170		43.856	9,826	25.900	1.001	104.96
	1240	, C	ASN	A	170		41.951	6.162	23.551	1.00	84.21
	1241	0	ASN	A	170		40.761	6.458	23.611	1.00	83.04
	1242	N	PRO	A	171		42.364	4.892	23.600	1.00	84.49

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	1243	CD	PRO A	171	43.716	4.318	23.698	1.00	86.08
	1244	CA	PRO A	171	41.335	3.862	23.753	1.00	84.63
	1245	СВ	PRO A	171	42.141	2.567	23.713	1.00	86.37
	1246	CG	PRO A	171	43.442	2.977	24.344	1.00	86.68
5	1247	С	PRO A	171	40.643	4.094	25.097	1.00	82.79
	1248	0	PRO A	171	39.598	3.513	25.392	1.00	82.76
	1249	N	GLY A	172	41.246	4.969	25.898	1.00	80.64
	1250	CA	GLY A	172	40.703	5.297	27.201	1.00	81.32
	1251	С	GLY A	172	39.764	6.488	27.163	1.00	81.29
10	1252	0	GLY, A	172	39.094	6.783	28.151	1.00	83.71
	1253	N	ASP A	173	39.721	7.182	26.030	1.00	79.07
	1254	CA	ASP A	173	38.842	8,336	25.870	1.00	75.74
	1255	CB	ASP A	173	39.260	9.159	24.651	1.00	85.90
	1256	CG	ASP A	173	40.356	10.146	24.968	1.00	90.56
15	1257	OD1	ASP. A	173	41.327	9.754	25.645	1.00	93.25
	1258	OD2	ASP A	173	40.248	11.313	24.536	1.00	92.57
	1259	C	ASP A	173	37.393	7.884	25.711	1.00	70.25
	1260	0	ASP A	173	36.464	8.691	25.777	1.00	68.50
	1261	N	ILE A	174	37.207	6.587	25.495	1.00	65.51
20	1262	CA	ILE A	174	35.876	6.023	25.340	1.00	60.45
	1263	СВ	ILE A	174	35.956	4.517	25.071	1.00	48.40
	1264	CG2			34.564	3.936	24.911		46.12
	1265	CG1	ILE A	174.	36.789		23.815		44.86
	1266	CD1		174	37.028		23.515		31.07
25	1267	С			35.086				58.37
	1268	0		174	35.421	5.712			58.27
	1269	N			34.042				55.65
	1270	CA			33.210				53.67
•	.1271	CB	THR A		33.526				57.15
30	1272	OG1				9.758	27.300		55.78
	1273				35.012				
	1274	С	THR A		31.751		27.264		52.38
	1275	0	THR A		31.454	7.143	26.089		52.43
٥.5	1276	N	GLU A		30.835				51.31
35			GLU A		29.423		27.858		48.46
	1278	CB	GLU A		28.555		29.114		37.51
	1279	CG	GLU A		28.426	6.080	29.688		45.01
	1280	CD	GLU A		27.472		30.858		45.89
40	1281		GLU A		26.435		30.834		42.92
40	1282		GLU A		27.757		31.792		34.90
		. C	GLU A		29.130		27.056		49.50
		0	GLU A		28.255				
	1285	N	GLU A	177	29.879	9.833	27.349	1.00	48.42

	1286	CA	GLU	A	177	29.721	11.092	26.645	1.00	48.94
	1287	СВ	GLU	A	177	30.646	12.153	27.253	1.00	63.07
	1288	CG	GLU	A	177	30.554	13.528	26.589	1.00	72.68
	1289	CD	GLU	A	177	31.888	14.267	26.554	1.00	76.09
5	1290	OE1	GLU	Α	177	31.912	15.439	26.114	1.00	77.97
	1291	OE2	GLU	Α	177	32.914	13.675	26.957	1.00	76.21
	1292	С	GLU	A	177	30.095	10.867	25.179	1.00	47.13
	1293	0	GLU	A	177	29.340	11.210	24.269	1.00	43.82
	1294	N	LEU	A	178	31.266	10.274	24.964	1.00	46.13
10	1295	CA	LEU	A	178	31.774	10.012	23.620	1.00	41.18
	1296	CB	LEU	A	178	33.167	9.373	23.704	1.00	31.24
	1297	CG	LEU	A	178	33.980	9.227	22.411	1.00	29.48
	1298	CD1	LEU	A	178	35.389	8.792	22.756	1.00	32.21
	1299	CD2	LEU	A	178	33.344	8.213	21.481	1.00	38.13
15	1300	С	LEU	A	178	30.839	9.128	22.800	1.00	41.26
	1301	0	LEU	A	178	30.355	9.551	21.752	1.00	44.23
	1302	N	ILE	A	179	30.596	7.905	23.271	1.00	37.47
	1303	CA	ILE	A	179	29.716	6.967	22.573	1.00	33.95
	1304	CB	ILE	Α	179	29.324	5.780	23.479	1.00	25.86
20	1305	CG2	ILE	A	179	28.262	4:950	22.807	1.00	27.50
	1306	CG1	ILE	A	179	30.545	4.905	23.762	1.00	24.58
	1307	CD1	ILE	A	179	30.292	3.777	24.748	1.00	16.92
	1308	С	ILE	A	179	28.443	7.673	22.127	1.00	36.09
	1309	0	ILE	A	179	27.885	7.374	21.069	1.00	36.52
25	1310	N	GLY	A	180	27.997	8.622	22.944	1.00	37.19
•	1311	CA	GLY	A	180	26.792	9.370	22.639	1.00	34.45
	1312	С	GLY	A	180	26.935	10.318	21.466	1.00	33.00
	1313	0	GLY	A	180	25.951	10.639	20.794	1.00	32.59
	1314	N	ASN	A	181	28.157	10.777	21.222	1.00	35.65
30	1315	CA	ASN	A	181	28.411	11.687	20.114	1.00	34.95
	1316	CB	ASN	A	181.	29.701	12.475	20.339	1.00	30.99
	1317	CG	ASN	A	181	29.654	13.321	21.578	1.00	27.11
	1318	OD1	ASN	A	181	28.679	14.027	21.818	1.00	30.62
	1319	ND2	ASN	A	181	30.715	13.268	22.372	1.00	34.99
35	1320	С	ASN	A	181	28.528	10.929	18.804	1.00	32.99
	1321	0	ASN	A	181	28.625	11.546	17.751	1.00	27.15
	1322	N	TYR	A	182	28.523	9.599	18.868	1.00	31.98
	1323	CA	TYR	A	182	28.645	8.778	17.670	1.00	30.09
	1324	CB	TYR	A	182	29.708	7.712	17.869	1.00	29.07
40		CG			182			17.726	1.00	30.62
	1326				182					31.56
					182	32.954	9.652	18.467	1.00	31.15
	1328	CD2	TYR	A	182	31.965	7.715	16.735	1.00	32.17

	1329	CE	2 TYR	A	182		33.287	8.156	16.606	1.00	29.49
	1330	CZ	TYR	A	182		33.774	9.123	17.473	1.00	30.88
	1331	ОН	TYR	A	182		35.079	9.548	17.337	1.00	38.87
	1332	С	TYR	Α	182		27.353	8.116	17.247	1.00	30.63
5	1333	0	TYR	A	182		27.316	7.417	16.238	1.00	27.81
	1334	N	LEU	A	183		26.296	8.331	18.023	1.00	33.68
	1335	CA	LEU	A	183		24.987	7.764	17.712	1.00	39.37
	1336	СВ	LEU	A	183		24.169	7.618	18.995	1.00	39.69
	1337	CG	LEU	A	183		24.813	6.778	20.096	1.00	35.29
. 10	1338	CD:	1 LEU	A	183		23.932	6.801	21.332	1.00	30.83
	1339	CD	2 LEU	A	183		25.016	5.361	19.602	1.00	36.26
	1340	С	LEU	A	183		24.250	8.671	16.715	1.00	40.34
	1341	0	LEU	A	183		24.537	9.865	16.626	1.00	39.87
	1342	N	PHE	A	184		23.302	8.110	15.969	1.00	38.84
15	1343	CA	PHE	A	184		22.556	8.890	14.984	1.00	37.83
	1344	CB	PHE	A	184		21.432	8.058	14.354	1.00	31.19
	1345	CG	PHE	Α	184		21.894	6.766	13.729	1.00	28.22
	1346	CDI	PHE	A	184		23.182	6.633	13.229	1.00	30.85
	1347	CD2	PHE	A	184		21.019	5.687	13.616	1.00	33.99
20	1348	CE1	PHE	A	184		23.587	5.443	12.627	1.00	24.17
	1349	CE2	PHE	A	184		21.417	4.493	13.013	1.00	21.76
	1350	CZ	PHE	A	184		22.699	4.372	12.519	1.00	18.36
	1351	С	PHE	A :	184		21.952	10.145	15.604	1.00	36.97
	1352	0	PHE .	A :	184		21.698	11.130	14.912	1.00	32.04
25	1353	N	THR .	A :	185		21.719	10.104	16.909	1.00	38.47
	1354	CA	THR .	A :	185		21.145	11.244	17.609	1:00	42.41
	1355	CB	THR I	A :	185		20.396	10.787	18.846	1.00	34.61
	1356	OG1	THR I	A :	185		21.213	9.862	19.570	1.00	41.28
	1357	CG2	THR I	A J	185		19.104	10.116	18.454	1.00	34.33
30	1358	С	THR I	A]	185		22.200	12.254	18.036	1.00	44.70
	1359	0	THR Z	A 1	185		21.946	13.086	18.905	1.00	41.53
	1360	N	GLN 2	A]	186		23.374	12.179	17.413	1.00	48.74
	1361	CA	GLN A	A]	186		24.494	13.072	17.711	1.00	49.59
	1362	CB	GLN A	A 1	186		25.775	12.501	17.132	1.00	45.10
35	1363	CG	GLN A	A 1	186		25.837	12.676	15.628	1.00	43.93
	1364	CD	GLN A	A 1	186		27.074	12.068	15,013	1.00	47.95
	1365	OE1	GLN A	A 1	186		27.201	10.848	14.920	1.00	50.02
	1366	NE2	GLN A	1	.86		28.000	12.918	14.593	1.00	38.99
	1367	С	GLN A	1	.86		24.279	14.451	17.097	1.00	51.53
40	1368	0	GLN F	1	.86		25.031	15.389	17.370	1.00	55'. 42
	1369	Ŋ	HIS F	1	.87		23.262	14.555	16.249	1.00	50.40
	1370	CA	HIS A	1	.87	•	22.934	15.800	15.568	1.00	49.57
	1371	СВ	HIS P	1	.87		22.157	15.474	14.295	1.00	42.89

	1372	ĊG	HIS	A	187		22.856	14.473	13.427	1.00	49.91
	1373	CD2			187		22.458			1.00	49.67
	1374	ND1	HIS	A	187		24.159	14.638	13.006	1.00	43.80
	1375	CE1	HIS	. A	1.87		24.536	13.578	12.311	1.00	48.87
5	1376	NE2	HIS	A	187		23.523	12.731	12.263	1.00	46.70
	1377	С	HIS	Α	187		22.145	16.735	16.469	1.00	52.33
	1378	0	HIS	A	187		22.402		16.513	1.00	53.97
	1379	N	LEU	A	188		21.187	16.182	17.196	1.00	54.52
	1380	CA	LEU	Α	188		20.391	16.982	18.109	1.00	51.83
10	1381	СВ	LEU	A	188		19.256	16.127	18.682	1.00	44.55
	1382	CG	LEU	A	188		18.288	15.528	17.650	1.00	47.65
	1383	CD1	LEU	Α	188		17.311	14.577	18.332	1.00	49.93
	1384	CD2	LEU	A	188	•	17.539	16.645	16.937	1.00	56.89
	1385	С	LEU	A	188		21.309	17.487	19.229	1.00	52.44
15	1386	0	TEU	A	188		22.248	16.802	19.628	1.00	53.35
	1387	N	PRO	Α	189		21.056	18.700	19.738	1.00	51.33
	1388	CD	PRO	A	189		19.887	19.538	19,434	1.00	51.94
	1389	CA	PRO	A	189		21.858	19.302	20.815	1.00	49.93
	1390.	СВ	PRO	A	189	٠.	21.115	20.601	21.115	1.00	51.02
20	1391	CG	PRO	A	189	•	19.701	20.275	20.733	1.00	52.36
	1392	С	PRO	A	189		21.978	18.411	22.045	1.00	46.59
	1393	0	PRO	A	189		21.001	17.807	22.476	1.00	45.97
	1394	N	LYS	Ä	190		23.169	18.351	22.625		42.50
		CA	•		190	٠٠, ١	23.390	17.495	23.782	1.00	39.80
25	1396	CB			190		24.672	17.885	24.526	1.00	36.33
	1397	CG	LYS				25.964	17.462			38.65
	1398	CD			190		27.169	17.626	24.750		42.37
	1399	CE	LYS				28.493	17.455	24,007		50.39
20	1400	NZ	LYS				28.687		23.447		58.82
30	1401	С	ΓÄS				22.256		24.789		39.26
	1402	0			190		21.827		25.075		39.95
	1403	N	ASP				21.751	18.475	25.328		40.10
	1404	CA	ASP				20.687		26.323		39.42
25	1405	CB			191		20.538	19.644	27.147		39.52
35	1406	CG	ASP				20.012	•	26.328		44.32
	1407		ASP				20.747	21.289	25.429		39.96
	1408		ASP				18.866	21.275	26.589		42.53
•	1409	C	ASP				19.323	17.893	25.777		39.16
40	1410		ASP				18.378				41.35
40	1411	N Cn	LEU				19.223	17.730	24.460		37.21
		CA	LEU				17.962	17.297	23.850		34.43
	1413	CB	LEU				17.484	18.337	22.815		26.76
	1414	CG	LEU	A	192		16.902	19.649	23.372	1.00	23.82

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               LEU A 192
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                              18.039 15.911
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               LEU A 192
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               ARG A 193
                              19.235 15.328
                                             23.193
                                                     1.00 30.50
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           CA
               ARG A 193
                              19.469 14.016 22.598 1.00 29.14
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           CB
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               ARG A 193
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               ARG A 193
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	1458	CD2	LEU	A	197	5.424	11.093	27.470	1.00	23.97
	1459	С	LEU	Α	197	9.100	9.292	25.987	1.00	24.32
	1460	0	LEU	Α	197	9.396	9.825	24.925	1.00	31.10
	1461	N	ILE	Α	198	8.752	8.018	26.082	1.00	25.23
5	1462	CA	ILE	Α	198	8.617	7.198	24.899	1.00	23.49
	1463	СВ	ILE	Α	198	9.663	6.079	24.843	1.00	16.92
	1464	CG2	ILE	Α	198	9.389	5.176	23.651	1.00	16.92
	1465	CG1	ILE	A	198	11.057	6.698	24.719	1.00	19.52
	1466	CD1	ILE	A	198	12.156	5.717	24.368	1.00	16.92
10	1467	С	ILE	A	198	7.214	6.621	24.894	1.00	26.00
•	1468	0	ILE	A	198	6.835	5.840	25.767	1.00	23.12
	1469	N .	ILE	A	199	6.448	7.056	23.901	1.00	30.16
	1470	CA	ILE	A	199	5.070	6.649	23.719	1.00	31.89
	1471	CB	ILE	A	199	4.275	7.798	23.061	1.00	31.40
15	1472	CG2	ILE	A	199	2.850	7.347	22.743	1.00	35.99
	1473	CG1	ILE	A	199	4.300	9.019	23.991	1.00	30.96
	1474	CD1	ILE	A	199	3.589	10.238	23.458	1.00	25.50
	1475	С	ILE	A	199	4.976	5.393	22.859	1.00	30.27
	1476	0	ILE	A	199	5.705	5.249	21.881	1.00	30.43
20	1477	N	ARG	A	200	4.087	4.483	23.246	1.00	29.84
	1478	CA	ARG	A	200	3.868	3.240	22.513	1.00	34.70
	1479	CB	ARG	A	200	4.567	2.070	23.214	1.00	38.24
	1480	CG	ARG	Α	200	4.553	0.763	22.420	1.00	38.39
	1481	CD	ARG	A	200	5.267	0.900	21.074	1.00	41.65
25	1482	NE	ARG	A	200	5.195	-0.302	20.234	1.00	34.53
	1483	CZ	ARG	A	200	5.923	-1.409	20.400	1.00	18.77
	1484	NH1	ARG	A	200	6.807	-1.510	21.385	1.00	16.92
	1485		ARG				-2.423			18.24
••	1486	С	ARG	A	200		3.011			35.76
30	1487	0	ARG	A	200	1.688	3.032	23.490	1.00	33.19
	1488	N			201		2.801		1.00	38.28
	1489	CA			201		2.610	21.078	1.00	37.05
	1490	CB			201	-0.118			1.00	16.92
25	1491				201		3.301		1.00	29.17
35	1492		THR			-0.060	4.947	20.321	1.00	19.67
	1493	С			201	-0.005		20.781	100	39.68
	1494	0			201		0.295		1.00	41.56
	1495	N			202		0.950		1.00	41.87
40	1496	CA	SER				-0.363			39.34
40	1497	CB	SER				-0.919	19.122		19.15
	1498	OG			202		-2.227			39.12
	. 1499	С					-1.421			40.05
	1500	0	SER	A	202	-2.303	-2.540	21.280	1.00	47.17

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	1501	N	GLY	A 203		-1.264	-1.080	22.634	1.00	38.45
	1502	CA	GLY A	A 203		-1.183	-2.038	23.729	1.00	37.08
	1503	С	GLY A	A 203	4	0.126	-2.815	23.773	1.00	35.70
	1504	0	GLY Z	A 203		0.305	-3.717	24.591	1.00	37.31
, 5	1505	N	GLU Z	204		1.048	-2.459	22.888	1.00	29.52
	1506	CA	GLU Z	A 204		2.336	-3.121	22.824	1.00	28.07
	1507	СВ	GLU Z	A 204	'	3.010	-2.835	21.484	1.00	26.30
	1508	CG	GLU Z	A 204		2.478	-3.664	20.328	1.00	48.79
	1509	CD	GLU A	A 204		2.437	-5.147.	20.655	1.00	50.97
10	1510	OE1	GLU A	A 204		1.371	-5.628	21.104	1.00	42.50
	1511	OE2	GLU A	A 204		3.470	-5.829	20.481	1.00	50.61
	1512	С	GLU A	A 204	•	3.249	-2.673	.23.942	1.00	29.34
	1513	0	GLU A	A 204	•	3.611	-1.507	24.014	1.00	34.97
	1514	N	LEU A	A 205		3.626	-3.604	24.811	1.00	24.91
15	1515	CA	LEU A	205	•	4.523	-3.307	25.925	1.00	25.98
	1516	CB	LEU A	A 205	•	3.943	-3.875	27.217	1.00	25.92
	1517	. CG	LĖU A	205		2.570	-3.293	27.561	1.00	23.50
	1518	CD1	LEU A	205		1.943	-4.043	28.704	100	16.92
	1519	CD2	LEU F	205		2.724	-1.837	27.917	1.00	30.67
20	1520	С	LEU F	205		5.905	-3.894	25.661	1.00	28.56
	1521	0	LEU F	205		6.494	-4.539	26.515	1.00	29.61
	1522	N	ARG A	206		6.418	-3.675	24.462	1.00	33.33
	1523	CA	ARG A	206	·	7.725	-4.191	24.108	1.00	37.25
	1524	СВ	ARG A	206	,	7.681	-4.932	22.766	1.00	42.74
25	1525	CG	ARG A	206		6.327	-5.519	22.392	1.00	40.30
	1526	CD	ARG A	206		6.381	-6.273	21.057	1.00	44.32
	1527	NE	ARG A	206		6.932	-5.469	19.960	1.00	65.13
	1528	CZ	ARG A	206		6.926	-5.836	18.677	1.00	69.76
	1529	NH1	ARG A	206		6.392	-6.999	18.325		76.09
30		NH2	ARG A	206		7.452	-5.045	17.741	1.00	74.71
	1531	С	ARG A	206		8.631	-2.991	23.963	1.00	42.39
	1532	0	ARG A			8.197	-1.852	24.144	1.00	42.90
	1533	N	LEU A			9.888	-3.247	23.625	1.00	44.87
	1534	CA	LEU A			10.834	-2.167	23.432	1.00	48.66
35		СВ	LEU A			12.136	-2.472	24.173	1.00	63.61
	1536	CG	LEU A			11.996	-2.330	25.693	1.00	70.49
	1537		LEU A			13.290	-2.729	26.376	1.00	76.92
	1538		LEU A		:	11.633	-0.885	26.044	1.00	75.21
	1539	С	LEU A	207		11.068	-1.969	21.939	1.00	47.29
40		0	LEU A		:	11.315	-0.849	21.484	1.00	47.01
	1541	N	SER A			10.971	-3.060	21.183	1.00	42.15
	1542	CA	SER A		:	11.139	-3.019	19.732	1.00	32.73
	1543	CB	SER A	208	1	10.005	-2.214	19.099	1.00	33.90

	1544	OG	SER	A	208		8.755	-2.556	19.666	1.00	24.12
	1545	С	SER	A	208		12.470	-2.441	19.263	1.00	28.39
	1546	0	SER	A	208		12.540	-1.821	18.198	1.00	29.45
	1547	N .	ASN	A	209		13.516	-2.629	20.064	1.00	26.85
5	1548	CA	ASN	A	209		14.861	-2.162	19.719	1.00	27.50
	1549	СВ	ASN	Α	209		15.404	-3.045	18.573	1.00	16.92
٠	1550	CG	ASN	A	209		16.864	-2.763	18.222	1.00	22.61
	1551	OD1	ASN	Α	209		17.693	-2.495	19.087	1.00	26.46
	1552	ND2	ASN	A	209		17.182	-2.857	16.939	1.00	20.95
10	1553	С	ASN	A	209		14.909	-0.675	19.348	1.00	32.21
	1554	0	ASN	Α	209		15.759	-0.241	18.573	1.00	34.11
	1555	N	PHE	Α	210		14.006	0.108	19.929	1.00	34.72
	1556	CA	PHE	Α	210		13.947	1.539	19.638	1.00	30.65
	1557	СВ	PHE	Α	210		12.484	2.000	19.582	1.00	21.62
15	1558	CG	PHE	Α	210		12.309	3.442	19.182	1.00	28.42
	1559	CD1	PHE	A	210		12.788	3.902	17.960	1.00	32.07
	1560	CD2	PHE	A	210		11.650	4.334	20.021	1.00	24.66
	1561	CE1	PHE	A	210		12.614	5.221	17.580	1.00	22.48
	1562	CE2	PHE	A	210		11.471	5.653	19.652	1.00	24.33
20	1563	CZ	PHE	A	210		11.955	6.099	18.427	1.00	18.91
	1564	С	PHE	Α	210		14.708	2.350	20.677	1.00	30.28
	1565	0	PHE	A	210		14.456	2.224	21.873	1.00	26.90
	1566	N	LEU	A	211		15.636	3.179	20.202	1.00	31.38
	1567	CA	LEU	A	211		16.460	4.030	21.060	1.00	30.02
25	1568	СВ	LEU	A	211		15.703	5.307	21.425	1.00	19.94
	1569	CG	LEU	A	211		15.642	6.415	20.381	1.00	17.90
	1570	CD1	LEU	A	211		15.015	7.668	21.000	1.00	17.79
	1571	CD2	LEU	A	211		17.051	6.710	19.886	1.00	28.12
	1572	С	LEU	A	211		16.940	3.356	22.344	1.00	33.52
30	1573	0	LEU	A	211		16.784	3.899	23.445	1.00	35.70
	1574	N	PRO	A	212		17,559	2.175	22.220	1.00	34.82
	1575	CD	PRO	A	212		18.096	1.603	20.977	1.00	34.05
	1576	CA	PRO	A	212		18.058	1.440	23.384	1.00	31.21
	1577	CB	PRO	A	212		18.807	0.283	22.748	1.00	30.61
35	1578	CG	PRO	A	212		19.305	0.881	21.473	1.00	33.84
	1579	С	PRO	A	212		18.941	2.279	24.317	1.00	28.88
	1580	0	PRO	A	212		18.734	2.286	25.529	1.00	28.95
	1581	N	TRP	A	213		19.911	2.991	23.747	1.00	32.89
	1582	CA	TRP	A	213		20.821	3.829	24.525	1.00	34.16
40	1583	СВ	TRP	A	213		22.076	4.133	23.699	1.00	36.50
	1584	CG	TRP	A	213	•	23.063	5.051	24.377	1.00	40.25
	1585	CD2	TRP	A	213		24.322	4.679	24.939	1.00	41.82
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	1589	NE:	1 TRP A 213	24.054	6.892	25.212	1.00 35.36
	1590	CZ	2 TRP A 213	26.170	5.851	26.074	1.00 41.79
5	1591	CZ.	3 TRP A 213	26.257	3.459	25.680	1.00 44.66
	1592	CH	2 TRP A 213	26.823	4.647	26.178	1.00 41.35
	1593	С	TRP A 213	20.210	5.143	25.045	1.00 31.31
	1594	0	TRP A 213	20.111	5.350	26.253	1.00 28.47
	1595	N	GLN A 214	19.814	6.031	24.139	1.00 29.42
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15	1601	NE2	2 GLN A 214	19.554	5.976	21.591	1.00 36.97
	1602	С	GLN A 214	18.041	7.180	25.484	1.00 26.22
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	1604	N	GLY A 215	17.229	6.153	25.271	1.00 24.50
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30	1616	CG	TYR A 217	18.180	7.000	32.935	1.00 16.92
	1617	CD1	TYR A 217	19.248	7.152	32.043	1.00 16.92
	1618	CE1	TYR A 217	20.558	6.868	32.436	1.00 16.92
	1619	CD2	TYR A 217	18.462	6.543	34.233	1.00 16.92
	1620	CE2	TYR A 217	19.768	6.256	34.632	1.00 16.92
35	1621	CZ	TYR A 217	20.808	6.423	33.730	1.00 16.92
	1622	OH	TYR A 217	22.103	6.168	34.115	1.00 16.92
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	1625	N	SER A 218	14.235	6.835	29.961	1.00 16.92
40	1626	CA	SER A 218	13.011	7.469	29.502	1.00 16.92
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15	1644	CD1	LEU	Α	220		9.297	1.	940	29.324	1.00	23.19
	1645	CD2	LEU	Α	220		9.707	3.9	943	27.887	1.00	16.92
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	1648	N	TYR	A	221		4.995	5.	633	28.311	1.00	23.31
20	1649	CA	TYR	A	221		3.550	5.	782	28.360	1.00	21.83
	1650	СВ	TYR	A	221		3.151	7.2	214	27.981	1.00	17.51
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30	1659	0	TYR	Α	221		3.383	4.	763	26.191	1.00	23.28
	1660	N	PHE	Α	222		2.066	3.9	932	27.799	1.00	24.60
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	1804	CD	LILE	A 23	39		2.717	16.967	25.299	1.00	28.23	
	1805	С	ILE	A 23	39		1.446	14.889	29.640	1.00	30.58	
5	1806	0	ILE	A.23	9		2.272	15.270	30,462	1.00	27.47	
	1807	N	LEÚ	A 24	0		0.165	14.745	29.934	1.00	30.48	
	1808	CA	LEU	A 24	0		-0.290	14.977	31.291	1.00	34.89	
	1809	СВ	LEU	A 24	0		-1.816	14.989	31.356	1.00	48.13	
	1810	CG	LEU	A 24	0		-2.523	16.290	30.988	1.00	43.96	
10	1811	CD1	LEU	A 24	0		-4.015	16.091	31.098	1.00	40.59	
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	1814	0	LEU	A 24	0	•	0.977	14:086	33.130	1.00	33.47	
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20		CA	TYR	A 24	2		4.018	12.297	32.036	1.00	49.44	•
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	1823	CG					6.049	13.671	31.333	1.00	37.89	
	1824	CD1					6.790	12.555	30.962	1.00	38.49	
~~	1825						8.173	12.630	30.821	1.00	37.07	
25	1826	CD2					6.724		31.557	1.00	33.74	
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	1833	CA	ASN A				5.936		35.296		65.83	
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35	1835 1836	CG OD1	ASN A				8.271	13.304	36.118		65.31	
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	1838		ASN A				8.643	13.607	37.354		65.91	
•	1839	C	ASN A				4.857	12.567	36.367		69.21	
	1840	0 N	ASN A				3.934	13.388	36.456		69.74	
40	1841	N CA	ARG A				4.971	11.499	37.159		68.62	
70	1842	CB	ARG A				4.010	11.193	38.221		71.05	
	1843	CB	ARG A				2.782	10.491	37.626		71.10	
	1844	CD	ARG A				1.687	10.186	38.633	1.00		
	1044	CD	ARG A	1 244	1		0.844	11.415	38.956	1.00	73.39	

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	86	CD1	ILE	В	25		12.368	-11.013	39.227	1.00 34.05
	87	С	ILE	B.	25		14.239	-6.516	38.179	1.00 34.24
	88	0	ILE	В	25	•	15.373	-6.557	38.655	1.00 40.45
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	91	СВ	ILE	В	26		13.754	-2.969	37.661	1.00 32.81
	92	CG2	ILE	В	26		14.178	-1.662	38.291	1.00 24.54
	93	CG1	ILE	В	26		14.567	-3.222	36.393	1.00 30.96
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	97	N	MET	В	27		13.553	-4.285	41.064	1.00 39.29
	98	CA	MET	В	27		12.756	-4.165	42.274	1.00 40.87
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	100	CG	MET	В	27		14.684	-5.327	43.596	1.00 33.29
	101	SD	MEI	B	27	•	15.109	-7.089	43.851	1.00 28.20
	102	CE	MET	' В	. 27		16.507	-7.243	42.803	1.00 29.62
	103	Ċ.	MET	В	27		12.687	-2.787	42.884	1.00 41.49
25	104	0	MET	·B	27		13.707	-2.156	43.172	1.00 44.33
	105	N	ASP	ıВ	28		11.448	-2.333	43.057	1.00 38.82
•	106	CA	ASP	В	28		11.135	-1.030	43.624	1.00 37.15
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35	114	CA	GLY	В	29		8.997	-0.237	46.639	1.00 31.71
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	118	CA	ASN	В	30		11.479	-1.259	49.322	1.00 34.55
40	119	СВ	ASN	В	30		12.982	-1.388	49.101	1.00 21.98
	120	CG	ASN	В	30		13.372	-2.739	48.528	1.00 23.62
	121	OD1	ASN	В	30		14.537	-2.979	48.222	1.00 20.30
	122	ND2	ASN	В	30		12.397	-3.634	48.392	1.00 20.74

	123	С	ASI	NВ	30	11.195	-0.224	50.395	1.00 38.93
	124	0	ASI	N B	30	10.527	-0.521	51.381	1.00 42.50
	125	N	GL:	ľΒ	31	11.693	0.992	50.199	1.00 38.13
	126	CA	GL:	ľΒ	31	11.481	2.053	51.173	1.00 37.44
5	127	С	GL	ζВ	31	10.033	2.484	51.353	1.00 37.86
	128	0	GL	ζВ	31	9.592	2.784	52.460	1.00 33.07
	129	N	ARC	3 B	32	9.291	2.532	50.256	1.00 41.86
	130	CA	ARG	3 B	32	7.890	2.920	50.300	1.00 43.79
	131	CB	ARG	B	32	7.331	2.969	48.876	1.00 50.98
10	132	CG	ARG	В	32	5.999	3.679	48.722	1.00 67.82
	133	CD	ARG	В	32	5.606	3.727	47.254	1.00 72.94
	134	NE	ARG	; в	32	4.186	4.006	47.062	1.00 79.64
	135	CZ	ARG	В	32	3.538	3.824	45.914	1.00 90.52
	136	NH1	ARG	В	32	4.186	3.365	44.849	1.00100.13
15	137	NH2	ARG	B	32	2.241	4.091	45.830	1.00 94.94
	138	С	ARG	В	32	7.171	1.867	51.135	1.00 41.07
	139	0	ARG	В	32	6.348	2.194	51.983	1.00 39.65
	140	N	TRE	В	33	7.510	0.605	50.885	1.00 39.29
	141	CA	TRE	В	33	6.948	-0.546	51.593	1.00 37.27
20	142	СВ	TRP	В	33	7.593	-1.834	51.081	1.00 28.51
	143	CG	TRP	В	33	7.184	-3.076	51.818	1.00 29.95
	144	CD2	TRP	В	33	7.882	-3.701	52.900	1.00 34.19
	145	CE2	TRP	В	33	7.137	-4.836	53.277	1.00 29.68
	146	CE3	TRP	В	33	9.065	-3.407	53.590	1.00 47.07
25	147		TRP		33	6.076	-3.835	51.592	1.00 35.81
	148		TRP		33	6.040	-4.896	52.462	1.00 31.40
	149		TRP		33	7.536	-5.684	54.316	1.00 27.96
	150		TRP		33	9.460		54.624	1.00 47.40
20	151		TRP		33				1.00 33.44
30	152	С	TRP		33		-0.428		1.00 35.31
	153	0	TRP		33	6.345	-0.603	53.918	1.00 35.16
	154	N	ALA		34	8.485	-0.151	53.408	1.00 30.64
	155	CA	ALA		34	8.907		54.791	1.00 26.94
25	156	CB	ALA		34			54.849	1.00 21.71
35	157	C	ALA		34			55.431	1.00 29.54
	158	0	ALA		34	7.619		56.487	1.00 30.57
	159	N CZ	LYS			8.397	2.359	54.773	1.00 30.23
	160	CA	LYS		35	7.851		55.263	1.00 32.86
40	161	CB	LYS		35	8.129	4.725	54.249	1.00 42.27
40	162	CG	LYS		35	8.577	6.048	54.859	1.00 58.11
	163	CD	LYS		35		7.167	53.834	1.00 74.59
	164	CE N7	LYS		35	7.059		53.311	1.00 85.25
	165	NZ	LYS	B	35	6.928	8.270	52.191	1.00 84.42

	166	С	LYS	В	35		6.353	3.523	55.551	1.00 38.17
	167	0	LYS	В	35		5.835	4.257	56.390	1.00 41.62
	168	N	LYS	В	36		5.652	2.624	54.870	1.00 41.65
	169	CA	LYS	B	36		4.219	2.498	55.094	1.00 43.49
5	170	СВ	LYS	В	36		3.519	1.935	53.850	1.00 52.09
	171	CG.	LYS	В	36		3.680	0.428	53.648	1.00 61.96
	172	CD	LYS	В	36		2.834	-0.098	52.468	1.00 65.82
	173	CE	LYS	В	36		2.974	-1.623	52.289	1.00 62.88
	174	NZ	LYS	В	36		2.084	-2.191	51.225	1.00 66.92
10	175	С	LYS	В	36		3.926	1.613	56.300	1.00 44.16
	176	0	LYS	В	36		2.857	1.706	56.895	1.00 46.34
	177	N	ARG	В	37		4.877	0.762	56.668	1.00 44.81
	178	CA	ARG	В	37		4.691	-0.129	57.803	1.00 46.91
	179	CB	ARG	В	37		5.305	-1.498	57.521	1.00 54.16
15	180	CG	ARG	В	37		4.652	-2.223	56.372	1.00 51.20
	181	CD	ARG	В	37		5.258	-3.588	56.141	1.00 52.57
	182	NE	ARG	В	37 .		4.915	-4.074	54.808	1.00 61.49
	183	CZ	ARG	В	37		3.675	-4.307	54.387	1.00 65.32
	184		ARG		37		2.653	-4.107	55.206	1.00 68.41
20	185		ARG		37		3.454	-4.713	53.140	1.00 59.01
	186	С	ARG		37		5.280	0.418	59.087	1.00 46.38
	187	0	ARG		37		5.519	-0.331	60.024	1.00 45.99
	. 188	N	MET		38		5.526	1.721	59.135	1.00 46.89
25	189	CA	MET		38		6.069	2.346	60.338	1.00 49.02
25	190	СВ	MET		38		5.216	1.987	61.564	1.00 46.95
	191	CG	MET		38		3.709	2.133	61.400	1.00 54.51
	192	SD	MET		38		3.148	3.835	61.214	1.00 62.23
	193	CE	MET		38		3.372	4.473	62.901	1.00 68.23
30	194 195	С 0	MET		38		7.517	1.960	60.652	1.00 49.28
50	196	N	MET		38		8.062	2.406	61.662	1.00 50.06
	197	CA	GLN GLN		39 39	•	8.148		59.821	1.00 49.00
	198	СВ	GLN		39		9.521 9.673	0.750	60.118	1.00 48.43
	199	CG	GLN		39				60.007	1.00 40.73
35	200	CD	GLN		39		8.855 8.846	-1.431	58.920	1.00 51.03
<i>55</i> ,	201		GLN		39		9.897	-2.945	59.070	1.00 54.07
	202		GLN		39		7.656	-3.586 -3.520	59.055	1.00 57.42
	203	C	GLN		39		10.589	1.455	59.225 59.298	1.00 38.98
	204		GLN		39		10.310	2.002		1.00 50.38
40	205	N	PRO		40		11.837	1.455	58.239 59.792	1.00 52.17 1.00 51.48
	206		PRO		40		12.308	0.759	61.004	
	207		PRO		40		12.958	2.100	59.108	1.00 50.84 1.00 49.78
	208		PRO		40		14.174	1.500	59.810	
				_				1.500	22.010	1.00 50.09

	209	CG	PRO	В	40		13.700	1.333	61.197	1.00 50.00
	210		PRC		40		12.980	1, 4		
	211	0	PRO		40		13.026		1	
	212	N	ARG	,в	41		12.941		·	1.00 44.90
5	213	CA			41		12.983			
	214	СВ	ARG	В	41	,	13.440			
	215	CG	ARG	В	41		13.629			
	216	CD	ARG	В	41		14.399			1.00 54.03
	217	NE	ARG	В	41		13.591			1.00 58.63
10	218	CZ	ARG	В	41		12.407		A company of	1.00 55.36
	219	NHI	. ARG	В	41		11.820	6.454	53.945	1.00 56.78
	220	NH2	ARG	В	41		11.816	8.145	52.397	1.00 41.95
	221	С	ARG	В	41		13.968	1.735	54.998	1.00 49.28
	. 222	0	ARG	В	41		13.690	0.912	54.124	1.00 51.60
15	223	N	VAL	В	42		15.110	1.713	55.674	1.00 46.21
	224	CA	VAL	В	42		16.178	0.757	55.390	1.00 45.66
	225	СВ	VAL	В	42		17.439	1.116	56.248	1.00 36.84
	226	CG1			42		17.513	0.234	57.479	1.00 30.96
00	227		VAL	В	42		18.706	1.024	55.403	1.00 31.91
20	228	С	VAL		42		15.831	-0.744	55:536	1.00 49.01
	229	0	VAL		42		16.461	-1.591	54.901	1.00 53.47
	230	N	PHE		43.		14.840	-1.078	56.360	1.00 46.72
	231	CA	PHE	'	43		14.455	-2.483	56.532	1.00 44.27
25	232	CB	PHE		43 "		13.378			1.00 37.66
25	233	CG	PHE		43		13.904	-2.642	59.017	1.00 36.94
	234	CD1	PHE		43	٠	15.273	-2.694		1.00 36.78
	235 236		PHE		43		13.018	-2.601	60.095	1.00 39.68
	237		PHE		43		15.750	-2.702	60.589	1.00 29.77
30	238				43		13.484		61.406	1.00 31.31
	239	C	PHE PHE		43 43					1.00 29.07
	240	0	PHE		43		·	-3.020	55.230	1.00 46.39
	241	N	GLY		44		13.083	-4.156	54.843	
	242	CA	GLY		44			-2.555	54.576	
35	243	С	GLY		44		13.381		52.426	
	244	0	GLY		44		12.959		51.766	1.00 40.10 1.00 40.32
	245	N	HIS		45			-2.969		
	246	CA	HIS		45		15.636		51.614	
	247	СВ	HIS	В	45		16.964		51.679	1.00 16.92
40	248	CG	HIS :		45		16.942	-1.595	50.981	1.00 28.29
	249	CD2	HIS :	В	45			-1.027	50.116	1.00 28.29
	250	ND1	HIS	В	45		15.934			1.00 34.82
	251	CE1	HIS	В	45		16.187	0.405		1.00 39.36

	252	NE	2 HIS	B	45		17.32	5 0.217	49.800	1.00	40.10
	253	С	HIS	В	45		15.79	8 -5.109	52.071	1.00	34.04
	254	0	HIS	В	45		15.83	7 -6.011	51.239	1.00	33.04
	255	N	LYS	'В	46		15.88	1 -5, 354	53.376	1.00	37.67
5	256	CA	LYS	, B	46		16.01	8 -6.734	53.821	1.00	36.56
	257	CB	LYS	В	46	•	16.05	2 -6.850	55.337	1.00	27.77
	258	CG	LYS	В	46	•	16.27	7 -8.288	55.800	1.00	36.67
	259	CD	LYS	В	46		16.52	-8.385	57.301	1.00	47.11
	260	CE	LYS	В	46	•	17.75	6 -7.581	57.721	1.00	45.30
10	261	NZ	LYS	В	46.		17.972	2 -7.582	59.198	1.00	54.67
	262	С	LYS	В	46		14.82	3 -7.497	53.296	1.00	35.24
	263	0	LYS	В	46		14.970	-8.572	52.714	1.00	34.48
	264	N	ALA	В	47		13.63	7 -6.929	53.497	1.00	34.22
	265	CA	ALA	В	47		12.404	7.552	53.019	1.00	33.65
15	266	CB	ALA	В	47	•	11.205	-6.669	53.346	.1.00	22.25
	267	С	ALA	B	47		12.493	3 -7.785	51.506	1.00	33.26
	268	0	ALA	В	47		12.057	-8.822	51.001	1.00	35.94
	269	N	GLY	В	48		13.048	-6.812	50.787	1.00	31.73
	270	CA	GLY	В	48		13.192	-6.973	49.360	1.00	31.22
20	271	С	GLY	В	48		13.881	-8.307	49.194	1.00	28.17
	272	0	GLY	В	48		13.376	-9.202	48.520	1.00	30.21
	273	N	MET	В	49		15,027	-8.448	49.848	1.00	26.41
	274	CA		В	49		15.801	-9.677	49.787	1.00	26.13
	275	CB	MET		49	•	17.005	-9.594	50.735		26.11
25	276	CG	MET	В	49	٠.	17.778	-10.911	50.907	1.00	31.14
	277	SD	MET.		49		19.315	-10.778	51.891	1.00	30.86
	278	CE	MET		49	4	18.675	-10.085	53.433	1.00	27.72
	279	С	MET		49			-10.894	50.128	1.00	26.86
20	280	0	MET		49		15.075	-11.936	49.493	1.00	25.74
30	281	N	GLU		50			-10.773			26.86
	282		GLU		50			-11.896	51.495	1.00	29.13
	283	CB	GLU		50			-11.527	52. 680 _.	1.00	35.38
	284	CG	GLU		50	:	13.166	-11.100	53.881	1.00	42.20
0.5	285	CD	GLU		50	:	L2.729	-11.778	55.161	1.00	55.85
35	286		GLU		50	-	L2.645	-13.028	55.166	1.00	54.70
	287		GLU		50	j	L2.483	-11.058	56.160	1.00	62.59
	288	С	GLU		50			-12.318	50.308	1.00	33.72
	289	0	GLU		50	1	.2.349	-13.491	49.937	1.00	40.50
40	290	N	ALA		51]	1.690	-11.363	49.700	1.00	30.97
40	291	CA	ALA		51	1	.0.863	-11.686	48.551	1.00	29.01
	292	CB	ALA		51			-10.470	48.108	1.00	33.60
	293	С	ALA		51			-12.187	47.414	1.00	28.16
	294	0	ALA	В	51	1	.1.291	-12.981	46.599	1.00	28.15

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	338	CE	LYS B	57		11.172	-20.838	48.431	1.00 55.23
	339	NZ	LYS B	57		11.143	-20.634	49.907	1.00 63.19
	340	С	LYS B	57		11.259	-20.335	43.523	1.00 44.75
	341	0	LYS B	5 7	•	11.263	-21.268	42.724	1.00 48.17
5	342	N	ALA B	58		10.198	-19.566	43.724	1.00 44.02
	343	CA	ALA B	58	٠.	8.952	-19.767	43.004	1.00 45.02
	344	СВ	ALA B	58		8.020	-18.608	43.269	1.00 31.05
· .	345	С	ALA B	58		9.216	-19.879	41.512	1.00 45.60
	346	0	ALA B	58	•	8.684	-20.754	40.841	1.00 47.49
10	347	N	ALA B	59		10.044	-18.978	40.999	1.00 43.55
	348	CA	ALA B	59		10.381	-18.949	39.581	1.00 44.39
	349	СВ	ALA B	59		11.187	-17.701	39.269	1.00 36.73
	350	С	ALA B	59		11.158	-20.182	39.164	1.00 48.03
	351	0	ALA B	59		11.173	-20.549	37.993	1.00 49.73
15	352	N	ASN B	60	•	11.809	-20.820	40.130	1.00 50.14
	353	CA	ASN B	60		12.600	-22.014	39.854	1.00 50.72
	354	СВ	ASN B	60		13.591	-22.261	40.998	1.00 56.81
•	355	CG	ASN B	60		14.507	-23.437	40.737	1.00 59.09
	356	OD1	ASN B	60		15.222	-23.477	39.738	1.00 50.39
20	357	ND2	ASN B	60		14.493	-24.403	41.645	1.00 68.87
	358	С	ASN B	60	ı	11.709	-23.238	39.660	1.00 48.92
	359	0	ASN B	60		11.954	-24.055	38.769	1.00 49.57
	360	N	LYS B	61		10.671	-23.353	40.489	1.00 44.16
	361	CA	LYS B	61	, ,	9.749	-24.477	40.403	1.00 42.23
25	362	CB	LYS B	61		8.810	-24.502	41.608	1.00 38.81
	363	CG	LYS. B	61	•	7.504	-23.750	41.382	1.00 49.61
	364	CD	LYS B	61		6.440	-24.149	42.397	1.00 61.71
	.365	CE	LYS B	61		5.080	-23.562	42.030	1.00 76.26
	366	NZ	LYS B	61		3.992	-23.993	42.958	1.00 77.30
30	367	С	LYS B	61		8.910	-24.362	39.143	1.00 41.26
	368	0	LYS B	61		8.286	-25.321	38.702	1.00 38.34
	369	N	LEU B	62		8.894	-23.170	38.570	1.00 43.33
	370	CA	LEU B	62		8.107	-22.921	37.379	1.00 40.43
	371	CB	LEU B	62		7.451	-21.541	37.478	1.00 41.05
35	372	CG	LEU B	62		6.153	-21.307	36.709	1.00 43.45
	373		LEU B	62		5.121	-22.374	37.061	1.00 49.97
	374	CD2	LEU B	62		5.626	-19.933	37.055	1.00 41.95
	375	С	LEU B	62		8.960	-23.026	36.124	1.00 37.78
	376	0	TEO B	62		8.490	-22.753	35.027	1.00 36.77
40	377	N	GLY B	63		10.219	-23.404	36.292	1.00 34.00
	378	CA	GLY B	63		11.087	-23.573	35.142	1.00 34.47
	379	С	GLY B	63		11.736	-22.368	34.483	1.00 34.70
	380	0	GLY B	63		12.311	-22.494	33.400	1.00 37.15

	381	N	VAL	В	64		11.649	-21.194	35.085	1.00	32.50
	382	CA	VAL		64			-20.051	34.475		33.85
	383	СВ	VAL		64			-18.780	35.297		38.31
	384	CG1	VAL	В	64			-17.652	34.783		
5	385	CĢ2	VAL	B	64		10.611	-18.390	35.224		30.49
	386	С	VAL	В	64		13.798	-20.376	34.449	1.00	32.11
	387	0 '	VAL	В	64		14.384	-20.691	35.478	1.00	35.71
	. 388	N	LYS	В	65	•	14.412	-20.317	33.277	1.00	30.11
	389	CA	LYS	B	65		15.830	-20.629	33.178	1.00	32.19
10	390	СВ	LYS	В	65		16.276	-20.642	31.720	1.00	34.45
•	391	CG	LYS	В	65		16.629	-22.024	31.194	1.00	28.19
	392	CD	LYS	В	65		15.416	-22.950	31.165	1,.00	32.70
	393	CE	LYS	В	65		15.722	-24.264	30.438	1.00	50.92
	394	NZ	LYS	В	65		16.090	-24.081	28.994	1.00	60.18
15	395	С	LYS	В	65		16.738	-19.695	33.963	1.00	32.24
	396 ·	0	LYS	В	6 5		17.634	-20.152	34.667	1.00	32.31
	397	N	VAL	В	66		16.515	-18.389	33.843	1.00	29.19
	398	CA	·VAL	В	66		17.342	-17.402	34.547	1.00	27.66
	399	СВ	VAL	В	66		18.647	-17.103	33.727	1.00	30.38
20	400	CG1	VAL	В	66		18.369	-17.285	32.254	1.00	29.01
	401	CG2	VAL	В	66		19.170	-15.681	34.002	1.00	16.92
	402	С	VAL	В	66		16.623	-16.087	34.846	1.00	22.57
	403	0	VAL	В	66		15.637	-15.758	34.199	1.00	18.50
	404	N	ILE	В	67		17.099	-15.360	35.855	1.00	23.89
25	405	CA	ILE	В	67		16.533	-14.054	36.196	1.00	31.24
٠.	406	CB	ILE	В	67		15.389	-14.129	37.259	1.00	30.49
	407	CG2	ILE	В	67		14.278	-15.044	36.761	1.00	32.00
	408		ILE		67		15.920	-14.612	38.604	1.00	35.49
20	409		ILE	В	67		14.844	-14.690	39.664	1.00	44.48
30	410	С	ILE		67		17.628	-13.112	36.685	1.00	32.32
	411	0	ILE	В	67		18.497	-13.490	37.483	1.00	36.35
	412	N	THR		68			-11.890	36.160	1.00	27.06
	413	CA	THR	В	68			-10.854	36.497	1.00	22.58
25	414	CB	THR		68			-10.256	35.239	1.00	20.26
35	415		THR		68			-11.283	34.524	1.00	31.06
	416		THR		68			-9.135	35.606	1.00	16.92
	417	С	THR		68		17.854	-9.756	37.281	1.00	26.08
	418		THR		68		17.017	-9.027	36.751	1.00	28.24
	419		VAL		69		18.210	-9.663	38.557	1.00	25.72
40	420		VAL		69		17.631		39.475	1.00	22.44
	421		VAL		69		17.459	-9.329	40.845	1.00	20.89
	422		VAL		69		16.430	-10.430	40.788	1.00	16.92
	423	CG2	VAL	В	69		18.784	-9.901	41.301	1.00	16.92

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-7.495 39.614
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                VAL B
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	467	N	GLU	В	75	24.340	4.360	39.900	1.00 63.63
	468	CA	GLU	В	75	23.804	5.621	40.394	1.00 66.15
	469	CB	GLU	В	75	22.783	6.165	39.389	1.00 75.90
	470	CG	GLU	В	75	22.350	7.593	39.651	1.00 93.53
5	471	CD	GLU	В	75	21.286	8.057	38.686	1.00103.81
	472	OE1	GLU	· B	75	20.236	7.384	38.593	1.00110.70
	473	OE2	GLU	В	75	21.500	9.094	38.023	1.00111.36
	474	С	GLU	В	75	23.168	5.533	41.779	1.00 66.40
	475	0	GLU	В	75	22.464	6.450	42.203	1.00 68.91
10	476	N	ASN	В	76	23.415	4.439	42.490	1.00 64.57
	477	CA	ASN	В	76·	22.845	4.281	43.825	1.00 59.63
	478	СВ	ASN	В	76	22.419	2.827	44.067	1.00 53.70
	479	CG	ASN	В	76	21.031	2.531	43.539	1.00 46.89
	480	OD1	ASN	В	76	20.101	3.305	43.752	1.00 50.66
15	481	ND2	ASN	В	76	20.880	1.402	42.861	1.00 40.20
	482	С	ASN	В	76	23.774	4.727	44.950	1.00 56.27
	483	0	ASŅ	В	76	23.319	4.953	46.071	1.00 55.41
	484	N	TRP	В	77	25.067	4.860	44.657	1.00 53.67
	485	CA	TRP	В	77	26.026	5.270	45.679	1.00 51.94
20	486	СВ	TRP	В	77	27.460	5.237	45.132	1.00 48.90
	487	CG	TRP	В	77	27.920	3.896	44.617	1.00 51.60
	488	CD2	TRP	В	77.	28.576	2.859	45.365	1.00 51.70
	489	CE2	TRP	В	77	28.839	1.797	44.467	1.00 52.11
	490	ĊE3	TRP	В	77, 2.	28.968	2.722;	46.706	1.00 43.86
25	491	CD1	TRP	В	77	27.812	3.431	43.338	1.00 52.12
	492	NE1	TRP	В	77 · ·	28.362	2.173	43.240	1.00 53.74
	493	CZ2	TRP	·B	77	29.476	0.616	44.865	1.00 43.91
	494	CZ3	TRP	В	77	29.603	1.540	47.101	1.00 37.41
	495	CH2	TRP	В	77	29.850	0.506	46.180	1.00 35.61
30	496	С	TRP	В	77	25.701	6.676	46.181	1.00 50.29
	497	0	TRP	В	77	26.194	7.112	47.226	1.00 54.30
	498	N	THR	В	78	24.858	7.369	45.428	1.00 46.30
	499	CA	THR	В	78	24.434	8.726	45.751	1.00 40.87
	500	CB	THR	В	78	23.518	9.268	44.646	1.00 40.94
35	501	OG1	THR	В	78	24.257	9.344	43.421	1.00 41.23
	502	CG2	THR	В	78	22.972	10.641	45.013	1.00 43.72
	503	С	THR	В	78	23.685	8.805	47.076	1.00 39.63
	504	0	THR	В	78	23.558	9.881	47.661	1.00 43.77
	505	N	ARG	В	79	23.194	7.662	47.548	1.00 33.93
40	506	CA	ARG	В	79	22.424	7.593	48.792	1.00 29.09
	507	CB	ARG	В	79	21.698	6.246	48.855	1.00 22.71
	508	CG	ARG	В	79	20.705	6.102	47.730	1.00 24.31
	509	CD	ARG	В	79	20.027	4.767	47.718	1.00 23.41

	510	NE	ARG	Ŕ	79	18.813	4.835	46.916	1.00	19.61
	511	CZ	ARG		79	17.945	3.839	46.780		25.88
	512		ARG		79	18.159	2.683	47.396		35.60
	513		ARG		79	16.858	4.004	•	•	23.97
5	514	С	ARG		79	23.217	7.830	•		31.63
	515	0	ARG		79	24.447	7.732	50.094	1.00	31.85
	516	N	PRO	В	80	22.513	8.167	51.17i	1.00	30.10
	517	CD	PRO	В	80	21.059	8.319	51.358	1.00	30.04
	518	CA	PRO	В	80	23.233	8.402	52.423	1.00	31.57
10	519	СВ	PRO	В	80,	22.113	8.754	53.414	1.00	29.71
	520	CG	PRO	В	80	20.904	8.083	52.840	1.00	29.28
	521	С	PRO	В	80	24.041	7.168	52.824	1.00	38.32
	522	0	PRO	В	80	23.487	6.083	53.011	1.00	42.42
	523	N	ASP	В	81	25.356	7.351	52.935	1.00	4,1.93
15	524	CA	ASP	B	81	26.284	6.284	53.299	,1.00	45.58
	525	СВ	ASP	В	81	27.427	6.850	54.150	1.00	63.07
	526	CG	ASP	В	81	28.116	8.043	53.504	1.00	67.38
	527		ASP		81	28.509	7.948	52.321	1.00	73.52
	528	OD2	ASP		81	28.274	9.075	54.189	1.00	72.51
.20	529	С	ASP		81	25.616	5.136	54.055	1.00	44.34
	530	0	ASP		81	25.671	3.984	53.626		45.14
	531	N	GLN		82	24,981	5.456	55.178		43.19
	532	CA	GLN		82	24.316	4.443	55.981	2.4 (4) 89	46.00
25	533	CB	GLN		82	23.492	5.110	57.076		45.03
25	534	CG	GLN		82	24.289	5.374	58.335		34.60
	535	CD	GLN.		82	24.607	4.099	59.104		16.92
	536		GLN		82	23.720	3.476	59.693		26.54
	537	NE2			82	25.875	3.703	59.098		16.92
30	538 539	С 0	GLN		82 82	23.448	3.473	55.187		47.51
50	540	N	GLN GLU			23.598	2.260	55.322		51.03
	541	CA	GLU		83	22.541 21.667	3.998	54.367		44.67
	542	CB	GLU		83	20.754	3.142 3.979	53.565 _. 52.664		37.68 35.83
	543	CG	GLU		83	19.621	3.191	52.003		39.43
35	544	CD	GLU		83		4.065	51.137		43.90
	545		GLU		83	17.556	3.666	50.877		48.19
	546		GLU :		83	19.176	5.149	50.706		48.89
	547	C	GLU I		83	22.517	2.232	52.700		32.89
	548		GLU		83	22.222	1.054	52.566		32.08
40	549		VAL 1		84	23.571	2.787	52.109		30.13
	550		VAL I		84	24.464	1.998	51.273		31.93
	551	СВ	VAL 1		84	25.503	2.884	50.546		35.84
	552		VAL I		84	26.379	2.025	49.640		39.26
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	553	CG2	VAI	В	84		24.792	3.946	49.722	1.00	34.99
	554	· C	IAV	ъΒ	84		25.177	1.016	52.196	1.00	33.63
	555	0	VAI	В	84		25.276	-0.178	51.903	1.00	34.73
	556	N	LYS	В	85		25.667	1.533	53.319	1.00	33.74
5	557	CA	LYS	B.	85		26.341	0.716	54.322	1.00	35.59
	558	СВ	LYS	В	85		26.496	1.544	55.612	1.00	48.55
	559	CG	LYS	В	85		26.571	0.767	56.928	1.00	59.03
	560	CD	LYS	В	85		27.942	0.170	57.196	1.00	67.33
	561	CE	LYS	В	85		27.943	-0.586	58.525	1.00	72.93
10	562	NZ	LYS	В	85		29.237	-1.290	58.785	1.00	68.29
	563	С	LYS	В	85		25.464	-0.525	54.545	1.00	33.73
	564	0	LYS	В	85		25.918	-1.655	54.380	1.00	32.87
	565	N	PHE	В	86		24.200	-0.280	54.882	1.00	34.91
	566	CA	PHE	В	86		23.192	-1.314	55.132	1.00	38.00
15	567	CB	PHE	В	86		21.840	-0.640	55.405	1.00	29.90
	568	CG	PHE	В	86		20.701	-1.`600	55.644	1.00	28.19
	569	CD1	PHE	В	86		20.164	-1.758	56.918	1.00	28.34
	570	CD2	PHE	В	86		20.112	-2.289	54.586	1.00	30.14
	571	CE1	PHE	В	86		19.052	-2.581	57.133	1.00	16.92
20	572	CE2	PHE	В	86		19.004	-3.114	54.792	1.00	31.79
	573	CZ	PHE	В	86		18.472	-3.258	56.067	1.00	23.42
	574	С	PHE	В	86		23.039	-2.310	53.982	1.00	41.33
	575	0	PHE	В	86		23.232	-3.512	54.170	1.00	44.39
	576	N	ILE	В	87	•	22.674	-1.811	52.800	1.00	42.94
25	577	CA	ILE	В	87		22.479	-2.661	51.624	1.00	44.91
	578	CB	ILE		87		22.225	-1.831	50.348	1.00	33.27
	579	CG2	ILE		87		21.956	-2.748	49.176	1.00	35.47
	580	CG1	ILE		87		21.018	-0.925	50.538	1.00	33.55
20	581	CD1	ILE		87		20.762	-0.027	49.357		
30	582	С	ILE		87		23.683	-3.552	51.354	1.00	49.45
	583	0	ILE		87			-4.774			51.81
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	585	CA	MET		88		26.064	-3.680	50.892		49.30
35	586	CB	MET		88		27.269		50.822		50.22
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	589 500	CE	MET		88		28.205	-3.366	47.823		32.68
	590 501	C	MET		88		26.352	-4.815	51.881		47.36
40	591	0	MET		88			-5.678	51.614		47.71
TU	592	N	ASN		89		25.676	-4.835	53.022		47.87
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	594 505	CB	ASN		89				55.400		59.69
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	596	OD1	ASN	В	89	27.61	1 -6.880	56.300	1.00	58.66
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5	772	CD	GL1	1 . E	3 i10		26.115	-17.355	36.147	1.00	53.12
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	774	NE2	GLN	IE	110	·	26.363	-16.329	35.331	1.00	66.31
	775	С	GLN	ŀE	110		25.825	-13.757·	39.615	1.00	35.02
	776	0	GLN	E	110		24.671	-13.423	39.890	1.00	36.09
10	77,7	N	MEI	' E	111.		26.821	-12.889	39.495	1.00	34.95
	778	CA	MEI	E	111		26.595	-11.463	39.665	1.00	38.29
	779	CB	MET	E	111		26.975	-11.034	41.091	1.00	54.75
	780	CG	MET	В	111		28.387	-11.398	41.561	1.00	63.44
	781	SD	MET	В	111		29.627	-10.096	41.304	1.00	75.55
15	782	CE	MET	. B	111		28.739	-8.620	41.902	1.00	63.96
	783	Ç	MET	В	111		27.358	-10.646	38.625	1.00	39.52
	784	0	MET	В	111		28.555	-10.836	38.435	1.00	42.08
	785	N	ILE	В	112		26.649	-9.743	37.948	1.00	39.74
	786	CA	ILE	В	112		27.241	-8.892	36.914	1.00	38.26
20	787	CB	ILE	В	112		26.406	-8.909	35.616	1.00	37.80
	788	CG2	ILE	В	112		26.317	-10.321	35.067	1.00	34.53
	789	CG1	ILE	В	112		25.017	-8.330	35.897	1.00	42.15
	790	CD1	ILE	В	112	2.	24.175	-8.130	34.672	1.00	40.41
	791	С	ILE	В	112		27.344			, 1.00	33.52
25	792	0			112		26.527	-6.947		1.00	28.71
	793	N			113		28.349	-6.743			30.89
	794	CA	•		113		28.521	-5.346		1.00	37.18
	795	С			113		29.944	-5.002			39.38
20	796	0			113		30.810	-5.869	37.513	1.00	38.55
30	797	N			114		30.178		37.789		
	798	CA			114		31.497		·		
	799	CB			114		31.548	-1.705			
	800	CG			114		31.688	-1.180	36.608		73.99
25	801	CD			114		30.510	-0.333	36.161		75.69
35	802		GLU				29.453	-0.904	35.805		75.15
	803		GLU					0.910	36.170	1.00	71.34
	804	С	GLU				31.753	-3.672	39.605	1.00	55.84
	805	0	GLU				31.591	-2.905	40.551	1.00	57.72
40	806	N			115		32.161	-4.925	39.745		57.14
40	807	CA			115		32.419	-5.530	41.042		58.68
	808	CB			115		32.550	-7.038	40.891	1.00	53.84
•	809	OG1					33.791	-7.332	40.244	1.00	53.59
	810	CG2	THR	В	115		31.409	-7.589	40.043	1.00	49.34

	*** 0 05	,040,0						
	811	С	THR I	3 115	33.675	-5.034	41.742	1.00 63.08
	812	. 0	THR E	3 115	34.010	-5.514	42.820	1.00 63.55
	813	N	ASP I	3 116	34.368	-4.070	41.147	1.00 67.68
	814	CA	ASP F	3 116	35.604	-3.566	41.736	1.00 72.55
5	815	СВ	ASP I	3 116	36.591	-3.200	40.623	1.00 76.81
	816	CG	ASP I	3 116	37.050	-4.415	39.831	1.00 82.99
	817	OD1	ASP I	3 116	36.200	-5.066	39.186	1.00 84.93
	818	OD2	ASP E	3 116	38.262	-4.723	39.860	1.00 75.26
	819	С	ASP E	3 116	35.487	-2.406	42.721	1.00 74.26
10	820	0 -	ASP E	3 116	36.442	-2.109	43.438	1.00 76.40
•	821	N	ARG E	3 117	34.332	-1.750	42.766	1.00 75.22
	822	CA	ARG E	3 117	34.145	-0.633	43.694	1.00 76.00
	823	CB	ARG E	3 117	33.392	0.514	43.009	1.00 91.55
	824	CG	ARG E	3 117	33.692	0.656	41.521	1.00106.10
15	825	CD	ARG E	3 117	32.965	1.850	40.908	1.00116.76
	826	NE	ARG E	3 117	32.740	1.680	39.472	1.00125.02
	827	CZ	ARG E		33.691	1.402	38.584	1.00129.50
	828		ARG E		34.951	1.258	38.975	1.00133.15
••	829		ARG E		33.381	1.264	37.300	1.00131.90
20	830	С	ARG B		33.348	-1.124	44.904	1.00 73.15
	831	0	ARG B		32.938	-0.339	45.765	1.00 75.52
	832	N	LEU B		33.145	-2.436		1.00 65.43
	833	CA	LEU B		32.390	-3.059	46.033	1.00 59.80
25	834	СВ	LEU B		31.834	-4.402	45.573	1.00 53.32
25	835	CG	LEU B		30.831	-4.440	44.427	1.00 51.22
	836	CD1			30.449	-5.893		1.00 43.14
	837		LEU B		29.599	-3.618	44.800	1.00 48.18
	838 839	С 0	LEU B		33.193	-3.303	47.294	1.00 55.75
30		N	LEU B		34.401	-3.496		1.00 56.56
30	841	CD	PRO B		32.516	-3.288	48.443	1.00 50.27
	842	CA	PRO B		31.151	-2.765	48.619	1.00 47.23
	843	CB	PRO B		33.158		49.735	
	844	CG	PRO B			-3.336		1.00 44.88
35	845	C	PRO B		31.170 33.680	-2.284 -4.065		1.00 43.34
55	846	0	PRO B		33.089	-4.965 -5.834	49.725	1.00 50.30
	847	N	LYS B		34.774	-5.223	49.090 50.427	1.00 51.90
	848	CA	LYS B		35.350	-6.564	50.427	1.00 52.17
	849	СВ	LYS B		36.628	-6.583	51.284	1.00 56.36
40	850	CG	LYS B		37.423	-7.877	51.156	1.00 63.53 1.00 63.00
-	851	CD	LYS B		38.405		52.305	1.00 63.00
	852	CE	LYS B		37.665		53.609	1.00 73.77
	853	NZ	LYS B		38.595	-8.673	54.713	1.00 69.29

	854	С	LYS	В	120		34.409	-7.647	50.967	1.00 55.74
	855	0	LYS	В	120		34.132	-8.625	50.272	1.00 56.30
	856	N	GLN	В	121		33.929	-7.479	52.196	1.00 55.41
	857	CA	GLN	В	.121		33.045	-8.470	52.791	1.00 54.91
5	858	СВ	GLN	В	121		32.572	-8.017	54.181	1.00 67.90
	859	CG	GLN	В	121		31.364	-7.087	54.199	1.00 74.11
	860	CD	GLN	В	121		31.694	-5.663	53.814	1.00 76.82
	861	OE1	GLN	В	121		30.807	-4.809	53.743	1.00 72.18
	862	NE2	GLN	В	121		32.971	-5.393	53.569	1.00 76.38
10	863	С	GLN	В	121		31.853	-8.729	51.881	1.00 52.21
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	865	N	THR	В	122		31.434	-7.695	51.159	1.00 49.30
	866	CA	THR	В	122	•	30.305	-7.807	50.238	1.00 43.48
	867	СВ	THR	В	122		29.897	-6.424	49.676	1.00 42.07
15	868	OG1	THR	В	122		29.714	-5.498	50.754	1.00 47.12
	869	CG2	THR	В	122		28.606	-6.536	48.875	1.00 43.57
	870	С	THR	В	122		30.719	-8.685	49.060	1.00 35.33
	871	0	THR	В	122		30.051	-9.667	48.715	1.00 27.53
	872	N	PHE	В	123		31.835	-8.307	48.449	1.00 33.58
20	873	CA	PHE	В	123		32.369	-9.018	47.304	1.00 35.10
	874	СВ	PHE	В	123		33.697	-8.407	46.879	1.00 37.63
	875	CG	PHE	В	123		34.247	-8.991	45.623	1.00 44.54
	876	CD1	PHE	В	123		33.554	-8.857	44.422	1.00 53.52
	877	CD2	PHE	В	123		35.450	-9.683	45.634	1.00 46.30
25.	878	CE1	PHE	В	123		34.054	-9.404	43.246	1.00 61.21
	879	CE2	PHE	В	123		35.960	-10.236	44.463	1.00 47.50
	880	CZ	PHE	В	123		35.261	-10.096	43.267	1.00 55.61
	881	С	PHE	В	123		32.581	-10.475	47.647	1.00 37.43
	882	0	PHE	В	123		31.977	-11.361	47.038	1.00 39.83
30	883	N	GLU	В	124		33.441	-10.716	48.629	1.00 37.07
	884	CA	GLU	В	124		33.742	-12.067	49.059	1.00 35.49
	885	СВ	GLU	В	124		34.570	-12.027	50.334	1.00 33.74
	886	CG	GLU	В	124		36.000	-11.595	50.089	1.00 34.11
	887	CD	GLU	В	124		36.734	-11.266	51.368	1.00 43.15
35	888	OE1	GLU	В	124		37.959	-11.020	51.299	1.00 48.58
	889	OE2	GLU	В	124		36.086	-11.246	52.440	1.00 60.13
-	890	С	GLU	В	124		32.481	-12.884	49.276	1.00 35.66
	891	0	GLU	В	124		32.440	-14.061	48.928	1.00 36.51
	892	N	ALA	В	125		31.449	-12.261	49.832	1.00 34.75
40	893	CA	ALA	В	125		30.195	-12.960	50.079	1.00 37.21
	894	CB	ALA	В	125		29.172	-12.005	50.655	1.00 34.20
	895	С	ALA	В	125		29.662	-13.570	48.793	1.00 40.90
	896	0	ALA	В	125		29.398	-14.771	48.719	1.00 44.51

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	942	C	GLU	В	131			30.948	-21.97	4	44.727	1.00	39.85
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	947	CG	LEU	В	132			27.441	-23.31	0 :	48.072	1.00	37.20
	948	CD1	LEU	В	132	•		28.184	-24.53	9.	48.543	1.00	40.73
10	949	CD2	LEU	В	132			26.740	-22.63	6	49.244	1.00	22.65
	950	С	LEU	В	132			28.390	-23.47	8	45.197	1.00	39.99
	951	0	LEU	В	132			28.364	-24.69	2	45.020	1.00	37.40
	952	N	THR	В	133			27.675	-22.62	4	44.475	1.00	43.53
	953	CA	THR	В	133			26.726	-23.05	7	43.454	1.00	43.29
15 ·	954	СВ	THR	B	133	•		25.540	-22.07	2	43.404	1.00	30.42
	955	OG1	THR	В	133			26.035	-20.72	5	43.410	1.00	32.09
	956	CG2	THR	В	133			24.640	-22.26	9	44.612	1.00	29.55
	957	С	THR	В	133			27.217	-23.30	3	42020	1.00	40.62
	958	0	THR	В	133			26.401	-23.58	0	41.140	1.00	37.19
20	959	N	LYS	В	134			28.527	-23.22	0	41.789	1.00	34.90
	960	CA	LYS	В	134	4		29.093	-23.44	8	40.454	1.00	36.42
	961	CB	LYS	В	134			30.563	-23.86	0	40.531	1.00	20.34
	962	ÇG	LYS	В	134			31.536	-22.77	5	40.932	1.00	39.12
	963	CD	LYS	В	134		,	32.983	-23.30	1 .	40.954	.1.00	44.98
25	964	CE	LYS.	В	134			33.173	-24.428	3 (41.970	1.00	44.22
	965	NZ	LYS	В	134			34.594	-24.85	7	42.103	1.00	45.46
	966	С	LYS	В	134			28.377	-24.53	4 :	39.668	1.00	44.36
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30	969	CA	ASN					28.002	-26.924	4 :	39.414	1.00	49.89
	970	CB	ASN					28.665	-28.213	3 :	39.909	1.00	51.24
	971	CG			135			30.165	-28.078	3 4	10.062	1.00	56.46
	972	OD1	ASN	В	135			30.824	-27.386	5 3	39.285	1.00	47.82
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35	974	С	ASN						-27.084		39.503	1.00	51.52
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	976	N	ASN						-26.084		10.019	1.00	51.08
	977		ASN					24.332	-26.206	5 4	10.094	1.00	50.58
	978		ASN					23.745	-25.176		11.056		44.34
40	979	CG	ASN					23.673	-25.693	3 4	12.480	1.00	37.46
	980	OD1							-25.085		13.337	1.00	26.38
	981	ND2							-26.823		12.738	1.00	42.23
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	1072	CA	GLY	В	148	24.973	0.390	34.849	1.00	35.29
5	1073	C ·	GLY	В	148	24.844	0.084	33.367	1.00	36.55
	1074	0	GLY	В	148	25.821	-0.266	32.713	1.00	34.11
	1075	N	GLY	В	149	23.635	0.216	32.836	1.00	35.88
	1076	CA	GLY	В	149	23.406	-0.053	31.428	1.00	35.86
	1077	С	GLY	В	149	24.445	0.531	30.489	1.00	33.73
10	1078	0	GLY	В	149	25.268	-0.194	29.924	1.00	34.86
	1079	N	ARG	В	150	24.411	1.845	30.308	1.00	29.19
	1080	CA	ARG	В	150	25.358	2.498	29.418	1.00	28.55
	1081	СВ	ARG	В	150	25.124	4.009	29.408	1.00	21.40
	1082	CG	ARG	В	150	23.737	4.438	28.938	1.00	21.80
15	1083	CD	ARG	В	150	23.659	5.946	28.778	1.00	16.92
	1084	NE	ARG	В	150	22.302	6.390	28.487	1.00	16.92
	1085	CZ	ARG	В	150	21.961	7.656	28.252	1.00	19.59
	1086	NH1	ARG	В	150	22.883	8.614	28.269	1.00	23.32
	1087	NH2	ARG	В	150	20.692	7.974	28.008	1.00	21.38
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	1091	CA	ALA	В	151	28.304	1.745	31.673	1.00	37.38
	1092	CB	ALA	В	151	28.254	, 1.688	33.194	1.00	52.48
25	1093	С	ALA	В	151	28.823	0.419	31.108	1.00	35.17
٠.	1094	0	ALA	В	151	29.959	0.345	30.635	1.00	31.19
	1095	N	GLU			27.990	-0.620	31.161	1.00	32.94
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	1099	CD			152	26.125	-5.100	30.149	1.00	22.76
	1100				152	25.001		30.160		
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25	1102	С			152	28.734		29.179	1.00	38.76
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	1105	CA	ILE			28.182	-1.146		1.00	38.31
	1106	СВ	ILE			27.053	-0.420	26.173	1.00	32.60
	1107				153	27.348	-0.418	24.692	1.00	35.83
40	1108		ILE			25.718		26.425		37.55
	1109					24.555				34.30
	1110	С	ILE			29.479			1.00	40.62
	1111	0	ILE	В	153	30.215	-0.747	25.729	1.00	37.23

	1112	N	THR B 154	29.747	0.631	27.446	1.00 45.36
	1113	CA	THR B 154	30.953	1.442	27.298	1.00 47.53
	1114	СВ	THR B 154	30.937	2.624	28.270	1.00 36.71
•	1115	OG	1 THR B 154	29.670	3.278	28.194	1.00 34.10
5	1116	CG:	2 THR B 154	32.016	3.617	27.910	1.00 31.30
	1117	C.	THR B 154	32.194	0.601	27.567	1.00 51.16
	1118	. 0	THR B 154	33.211	0.732	26.885	1.00 50.52
	1119	N	GLN B 155	32.099	-0.260	28.572	1.00 55.38
	1120	CA	GLN B 155	33.192	-1.143	28.946	1.00 57.33
, 10	1121	СВ	GLN B 155	32.855	-1.851	30.264	1.00 67.23
	1122	CG	GLN B 155	33.707	-3.068	30.590	1.00 83.16
	1123	CD	GLN B 155	33.045	-4.380	30.180	1.00 90.67
	1124	OE:	l GLN B 155	33.604	-5.461	30.385	1.00 95.55
	1125	NE2	2 GLN B 155	31.849	-4.291	29.603	1.00 94.98
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	1133	N	LEU B 157	32.500	-1.725	24.766	1.00 53.20
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,	1135	CB	LEU B 157	32.004	0.286	23.480	1.00 59.88
25 .	1136	CG	LEU B 157	32.116	1.171	22.238	1.00 68.36
	1137		LEU B 157	30.749	1.785	21.941	1.00 66.20
	1138	CD2	LEU B 157	33.190	2.240	22.442	1.00 73.25
	1139	С	LEU B 157	34.376	-0.535	23.711	1.00 53.24
20	1140	0	LEU B 157	35.027	-0.250	22.709	1.00 53.64
30	1141	N	LYS B 158	34.889	-0.522	24.935	1.00 48.90
	1142		LYS B 158		-0.156	25.196	1.00 43.03
	1143	CB	LYS B 158	36.395	0.368	26.632	1.00 51.76
	1144	CG	LYS B 158	37.738	0.976	27.006	1.00 50.73
2.5	1145	CD	LYS B 158	37.553	2.108	28.020	1.00 59.64
35	1146	CE	LYS B 158	36.717	1.678	29.233	1.00 62.25
	1147	NZ	LYS B 158	36.406	2.801	30.175	1.00 58.23
	1148	С	LYS B 158	37.174	-1.374	24.983	1.00 38.44
	1149	0	LYS B 158	38.192	-1.288	24.304	1.00 36.00
40	1150	N	LEU B 159	36.784	-2.505	25.566	1.00 39.17
40	1151	CA	LEU B 159	37.530	-3.755	25.432	1.00 39.21
	1152	CB	LEU B 159	36.780		26,116	1.00 46.03
	1153	CG	LEU B 159	36.840		27.635	1.00 49.65
	1154	CD1	LEU B 159	35.775	-5.991	28.124	1.00 52.44

	1155	CD2	LEU	В	159		38.222	-5.492	28.034	1.00	50.53
	1156	С	LEU	В	159		37.729	-4.121	23.964	1.00	38.04
	1157	0	LEU	В	159		, 38.792	-4.599	23.576	1.00	32.72
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	1160	CB	ILE	В	160		35.382	-4.045	21.062	1.00	29.65
	1161	CG2	! ILE	В	160		35.493	-4.272	19.559	1.00	21.54
	1162	CG1	ILE	В	160		34.383	-5.027	21.668	1.00	33.17
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10	1164	С	ILE	В	160		37.767	-3.303	21.042	1.00	42.75
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	1166	N	SER	В	161		37.662	-2.001	21.283	1.00	47.98
	1167	CA	SER	В	161		38.593	-1.055	20.678	1.00	52.98
	1168	CB	SER	В	161		38.154	0.387	20.942	1.00	51.83
15	1169	OG	SER	В	161		36.966	0.699	20.235	1.00	47.45
	1170	С	SER	В	161		39.987	-1.270	21.244	1.00	54.93
	1171	0	SER	В	161	•	40.862	-0.420	21.103	1.00	59.36
	1172	N	GLN	В	162		40.183	-2.407	21.902	1.00	54.75
	1173	CA	GLN	В	162		41.471	-2.748	22.480	1.00	57.55
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	1175	CG	GLN	В	162		42.644	-3.337	24.667	1.00	59.30
	1176	CD			162		43.554	-2.129	24.738	1.00	61.11
	1177		GLN				43.922	-1.555	23.716	1.00	65.88
	1178	NE2	GLN	B	162	٠.	.43.923	-1.738	25.951	1.00	72.94
25	1179	С	GLN				41.989	-3.987	21.764	1.00	60.23
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	1182	CA	ASP				41.482	-6.208	20.925	1.00	59.20
20	1183	СВ	ASP				40.345	-7.229	21.037	1.00	59.79
30	1184	CG	ASP					-7.668		1.00	63.02
	1185				163		40.045	-6.796		1.00	72.81
	1186		ASP				39.924	-8.883	22.701	1.00	61.86
	1187	С	ASP				41.730	-5.850	19.459	1.00	57.70
25	1188	0	ASP				42.537	-6.482	18.782	1.00	55.82
35	1189	N	VAL				41.025	-4.828	18.981	1.00	57.73
	1190	CA	VAL				41.160	-4.365	17.606	1.00	59.37
	1191	CB	VAL				40.087	-3.332	17.249	1.00	55.59
	1192		VAL					-2.753	15.865	1.00	47.40
40	1193		VAL					-3.975		1.00	51.18
40	1194	С	VAL				42.504	-3.694	17.443		62.08
	1195	0	VAL					-3.914			65.19
	1196	N	LEU					-2.853			63.92
	1197	CA	LEU	В	165		44.104	-2.142	18.394	1.00	62.86

	1198	CB	LEU'B 165	44.143	3 -1.140	19.547	1.00 45.47
	1199	CG	LEU B 165	45.282	2 -0.128	19.554	1.00 40.70
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5	1202	С	LEU B 165	45.218	3 -3.174	18.526	1.00 63.35
	1203	0	LEU B 165	46.195	-3.143	17.778	1.00 63.16
	1204	N	ASP B 166	45.053	3 -4.099	19.466	1.00 64.85
	1205	CA	ASP B 166	46.029	-5.161	19.678	1.00 65.80
	1206	СВ	ASP B 166	45.736	5 -5.902	20.983	1.00 71.82
10	1207	CG	ASP B 166	46.139	-5.108	22.204	1.00 70.86
	1208	OD	1 ASP B 166	45.691	-3.950	22.338	1.00 65.25
	1209	OD.	2 ASP B 166	46.904	-5,642	.23.035	1.00 80.37
	1210	С	ASP B 166	45.977	-6.145	18.514	1.00 66.21
	1211		ASP B 166	46.435	-7.282	18.625	1.00 ,65.89
15	1212		ALA B 167	45.408	-5.691	17.400	1.00 66.17
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	1214		ALA B 167	46.612	-6.539	15.449	1.00 63.12
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•	1218	CA	LYS B 168	42.891		16.935	1.00 70.73
	1219	CB	LYS B 168	42.391		18.371	1.00 55.74
	1220	CG	LYS B 168	43.483		19.384	1.00 43.98
25	1221	CD	LYS B 168		-10.035	20.709	1.00 50.77
23	1222	CE	LYS B 168	·	-10.341	21.712	1.00 54.71
	1223 1224	NZ	LYS B 168	44.917		21.875	1.00 56.54
	1224	C	LYS B 168	41.723		15.993	1.00 74.61
	1226	O N	LYS B 168		-10.448	15.137	1.00 79.29
30	1227	CA	ILE B 169 ILE B 169	40.709		16.160	1.00 75.01
	1228	CB	ILE B 169	39.541	-8.796 -8.822	15.307	1.00 77.20
	1229		ILE B 169		-10.003	16.137	
	1230		ILE B 169	38.051	-7.519	17.095 16.922	1.00 64.44
	1231		ILE B 169	39.064	-7.319	18.014	1.00 67.21
35	1232	С	ILE B 169	39.571	-7.577	14.400	1.00 62.39
	1233	0	ILE B 169	39.866	-6.470	14.400	1.00 81.65 1.00 82.71
	1234	N	ASN B 170	39.298	-7.792	13.116	1.00 82.71
	1235	CA	ASN B 170	39.299	-6.699	12.153	1.00 86.01
	1236	СВ	ASN B 170	38.780	-7.160	10.781	1.00 88.01
40	1237	CG	ASN B 170	39.291	-8.540	10.382	1.00105.24
	1238		ASN B 170	40.415	-8.921	10.713	1.00109.37
	1239		ASN B 170	38.466		9.651	1.00103.37
	1240	С	ASN B 170	38.361	-5.641	12.695	1.00 84.21
						~~.033	1.00 04.21

	1241	0	ASN	в 170		37.397	-5.960	13.385	1.00	83.04
	1242	N	PRO	B 171		38.630	-4.364	12.407	1.00	84.49
	1243	CD	PRO	в 171		39.617	-3.766	11.493	1.00	86.08
	1244	CA	PRO	в 171		37.708	-3.355	12.931	1.00	84.63
5	1245	CB	PRO	в 171		38.340	-2.045	12.469	1.00	86.37
	1246	CG	PRO	в 171		38.976	-2.436	11.164	1.00	86.68
	1247	C	PRO	в 171		36.336	-3.610	12.306	1.00	82.79
	1248	0	PRO	в 171		35.323	-3.051	12.726	1.00	82.76
	1249	N	GLY	B 172		36.328	-4.480	11.299	1.00	80.64
10	1250	CA	GLY	в 172		35.100	-4.828	10.613	1.00	81.32
	1251	С	GLY	В 172		34.411	-6.036	11.219	1.00	81.29
	1252	0	GLY	в 172		33.278	-6.351	10.859	1.00	83.71
	1253	N	ASP :	в 173	-	35.094	-6.722	12.130	1.00	79.07
٠	1254	CA	ASP	в 173		34.527	-7.890	12.795	1.00	75.74
15	1255	CB	ASP 1	В 173		35.627	-8.696	13.487	1.00	85.90
	1256	CG	ASP 1	В 173		36.308	-9.665	12.553	1.00	90.56
	1257		ASP 1			36.641	-9.260	11.421	1.00	93.25
	1258	OD2	ASP 1			36.514	-10.830	12.952	1.00	92.57
20	1259	C	ASP I	B 173		.33.481	-7.464	13.822	1.00	70.25
20	1260	0	ASP I			32.727	-8.288	14.343		68.50
	1261	N	ILE I			33.444	-6.169	14.114		65.51
	1262	CA	ILE E			32.486	-5.628	15.064		60.45
	1263	CB	ILE E			32.687	-4.119	15.234		48.40
			ILE E				-3.562	16.226		46.12
25	1265	CG1				34.115	-3.851			44.86
	1266	CD1				34.461	-2.387	15.797		31.07
	1267	C	ILE E			31.077	-5.886	14.549		58.37
	1268 1269	O N	ILE E			30.679	-5.344	13.524		58.27
30	1270	N CA	THR E			30.327	-6.719	15.261		55.65
30	1271	CB				28.964	-7.043	14.869		53.67
	1272		THR E			28.897	-8.435	14.236		57.15
	1273		THR E			29.168 29.932	-9.429	15.230		55.78
	1274	C C	THR E			28.084	-8.560 -7.033	13.145		49.80
35	1275	0	THR E			28.577	-7.032 -6.835	16.110 17.217		52.38
	1276	N	GLU B			26.784	-7.232	15.938		52.43 51.31
	1277	CA	GLU B			25.895	-7.261	17.089		
	1278	СВ	GLU B			24.434	-7.240	16.643		48.46 37.51
	1279	CG	GLU B			23.950	-5.856	16.281		45.01
40	1280	CD	GLU B			22.474	-5.813	15.956		45.89
	1281		GLU B			21.690		16.615		42.92
	1282		GLU B				-5.036	15.051		34.90
	1283	С	GLU B			26.187	-8.519	17.893	-	49.50

	1284	0	GLU	B 176	26.038	8 -8.544	19.113	1.00 49.76
	1285	N	GLU	в 177	26.613	-9.563	17.192	1.00 48.42
	1286	CA	GLU	в 177	26.950	-10.820	17.836	1.00 48.94
	1287	СВ	GLU	в 177	27.318	-11.868	16.779	1.00 63.07
5	1288	CG	GLU	в 177	27.685	-13.239	17.350	1.00 72.68
	1289	CD	GLU	в 177	28.766	-13.953	16.545	1.00 76.09
	1290	OE	1 GLU	в 177	29.081	-15.121	16.869	1.00 77.97
	1291	OE	2 GLU	в 177	29.309	-13.346	15.595	1.00 76.21
	1292	С	GLU	в 177	28.149	-10.576	18.754	1.00 47.13
. 10	1293	0	GLU	В 177	28.129	-10.926	19.934	1.00 43.82
	1294	N	LEU	B 178	29.189	9.960	18.199	1.00 46.13
	1295	CA	LEU	B 178	30.416	-9.678	18.938	1.00 41.18
	1296	CB	LEU	в 178	31.444	-9.015	18.011	1.00 31.24
	1297			В 178	32.881		18.521	1.00 29.48
15	1298		l LEU		33.762		17.378	1.00 32.21
	1299		2 LEU :	B 178		-7.834	19.650	1.00 38.13
	1300	С		B 178	30.176		20.166	1.00 41.26
	1301	0		3 178	30.455		21.286	1.00 44.23
20	1302	N		3 179	29.669		19.954	1.00 37.47
20	1303	CA		3 179	29.395		21.053	1.00 33.95
	1304	CB		3 179	28.502		20.592	1.00 25.86
	1305		? ILE E		28.071		21.783	1.00 27.50
i	. 1306		ILE E		29.267	.*	19.617	1.00 24.58
25	1307 1308	C	ILE E		28.434		19.007	1.00 16.92
23,	1309	0	ILE E		28.687			1.00 36.09
	1310	N	GLY E		28.901 27.849	-7.093 -8.353	23.367	1.00 36.52
	1311	CA	GLY E		27.108	-0.333 -9.120	21.821	1.00 37.19
	1312	С	GLY E			-10.057	22.804	1.00 34.45
30	1313	0	GLY E			-10.390	24.766	1.00 33.00 1.00 32.59
	1314	N	ASN E					1.00 32.39
	1315	CA	ASN B			-11.388		1.00 33.05
	1316	СВ	ASN B			-12.153	22.784	1.00 34.93
	1317	CG	ASN B			-13.010		1.00 27.11
35	1318	OD1	ASN B			-13.735		1.00 27.11
	1319		ASN B			-12.943		1.00 34.99
	1320	С	ASN B	181		-10.617	24.724	1.00 32.99
	1321	0	ASN B	181			25.486	1.00 27.15
	1322	N	TYR B	182		-9.288	24.684	1.00 31.98
40	1323	CA	TYR B	182	31.634	-8.456	25.552	1.00 30.09
	1324	СВ	TYR B	182	32.323	-7.372	24.742	1.00 29.07
	1325	CG	TYR B	182	33.529	-7.857	23.974	1.00 30.62
	1326	CD1	TYR B	182	33.411	-8.828	22.976	1.00 31.56

	1327	CE1	TYR	., В	182	34.533	-9.256	22.247	1.00	31.15
	1328	CD2	TYR	. B	182	34.796	-7.325	24.229	1.00	32.17
	1329	CE2	TYR	В	182	35.921	-7.740	23.507	1.00	29.49
	1330	CZ	TYŖ	В	182	35.783	-8.705	22.520	1.00	30.88
5	1331	ОН	TYR	В	182	36.898	-9.105	21,814	1.00	38.87
	1332	С	TYŔ	В	182.	30.871	-7.814	26.689	1.00	30.63
	1333	0	TYR	В	182	31.455	-7.108	27.507	1.00	27.81
	1334	N	LEU	В	183	29.565	-8.055	26.736	1.00	33.68
	1335	CA	LEU	· в	183 .	28.722	-7.510	27.795	1.00	39.37
10	1336	СВ	LEU	В	183	27.281	-7.389	27.298	1.00	39.69
	1337	CG	LEU	٠B	183	27.086	-6.546	26.040	1.00	35.29
	1338	CD1	LEU	В	183 .	25.629	-6.594	25.618	1.00	30.83
	1339	CD2	LEU	В	183	27.525	-5:121	26.308	1.00	36.26
	1340	С	LEU	В	183	28.780	-8.422	29.030	1.00	40.34
15	1341	0	LEU	В	183,	29.084	-9.610	28.915	1.00	39.87
	1342	N	PHE	В	184	28.490	- 7.873	30.206	1.00	38.84
	1343	CA	PHE	В	184	28.532	-8.659	31.437	1.00	37.83
•	1344	СВ	PHE	В	184	28.026	-7.843	32.633	1.00	31.19
	1345	CG	PHE	В	184	28.751	-6.538	32.843	1.00	28.22
20	1346	CD1	PHE	В	184	30.068	-6.377	32.436	1.00	30.85
	1347	CD2	PHE	В	184	28.115	-5.474	33.481	1.00	33.99
	1348	CE1	PHE	В	184	30.736	-5.175	32.663	1.00	24.17
	1349	CE2	PHE	В	184	28.778	-4.268	33.713	1.00	21.76
	1350	CZ	PHE	В	184	30.087	-4:120	33.305	1.00	18.36
25	1351	С	PHE	В	184	27.697	-9.929	31.319	1.00	36.97
	1352	0	PHE	В	184	27.947	-10.914	32.014	1.00	32.04
	1353	N	THR	В	185	26.704	-9.903	30.441	1.00	38.47
	1354	CA	THR	В	185	25.841	-11.059	30.243	1.00	42.41
	1355	СВ	THR	В	185	24.478	-10.625	29.741	1.00	34.61
30	1356	OG1	THR	В	185	24.651	-9.691	28.671	1.00	41.28
	1357	CG2	THR	В	185	23.696	-9.975	30.853	1.00	34.33
	1358	С	THR	В	185	26.423	-12.052	29.248	1.00	44.70
	1359	0	THR	В	185	25.700	-12.896	28.720	1.00	41.53
	1360	N	GLN	В	186	27.728	-11.951	29.008	1.00	48.74
35	1361	CA	GLN	В	186	28.438	-12.826	28.074	1.00	49.59
	1362	CB	GLN	В	186	29.790	-12.227	27.736	1.00	45.10
	1363	CG					-12.389		1.00	43.93
	1364	CD	GLN	В	186	32.116	-11.753	28.593	1.00	47.95
	1365						-10.530	28.593	1.00	50.02
40	1366	NE2	GLN	В	186	33.119	-12.583	28.342	1.00	38.99
	1367							28.682		51.53
	1368	0	GLN	В	186			27.996	1.00	55.42
	1369	N	HIS	В	187	28.409	-14.320	29.977	1.00	50.40

	1370	CA	HIS	S B	3 187		28.598	-15.565	30.708	1.00	49.57
	1371	СВ	HIS	SE	3 187		28.773	3 -15.243	32.190	1.00	42.89
	1372	CG	HIS	3 E	3 187		29.841	-14.223	32.442	1.00	49.91
	1373	CD	2 HIS	3 I	3 187		29.801	-13.022	33.068	1.00	49.67
5	1374	ND:	l HIS	5 E	3 187		31.127	7 -14.361	31.962	1.00	43.80
	1375	CE	1 HIS	5 E	3 187		31.833	3 -13.289	32.278	1.00	48.87
	1376	NE	2 HIS	S E	3 187	•	31.053	3 -12.460	32.949	1.00	46.70
	1377	С	HIS	S E	3 187		27.439	-16.521	30.487	1.00	52.33
	1378	0	HIS	S E	3 187	•	27.636	5 -17.718	30.286	1.00	53.97
10	1379	N	LEU	JE	188		26.226	-15.992	30.514	1.00	54.52
	1380	CA	LEU	JE	188		25.051	-16.813	30.289	1.00	51.83
	1381	CB	LEU	JE	188		23.789	-15.984	30.549	1.00	44.55
	1382	CG	LEU	JE	188		23.659	-15.395	31.962	1.00	47.65
	1383	CD1	LEC	JE	188		22.452	-14.467	32.039	1.00	49.93
15	1384	CD2	LEU	J _. B	188	•	23.537	-16.520	32.980	1.00	56.89
	1385	С	LEU	JB	188		25.085	-17.310	28.838	1.00	52.44
	1386	.0	LEU	B	188		25.560	-16.611	27.946	1.00	53.35
	1387	N	PRO	B	189		24.594	-18.532	28.590	100	51.33
	1388	CD	PRO	В	189		23.882	-19.388	29.549	1.00	51.94
20	1389	CA	PRO	В	189		24.565	-19.127	27.244	1.00	49.93
•	1390	CB	PRO	В	189		23.822	-20.442	27.463	1.00	51.02
	1391	CG	PRO	В	189		22.944	-20.139	28.642	1.00	52.36
	1392	C .			189	٠	23.878	-18.244	26.210	1.00	46.59
~ -	1393	0			189	•		-17.661	26.482	1.00	45.97
25	1394	N						-18.166	25.016	1.00	42.50
	1395	CA			190			-17.315	23.977		39.80
	1396	CB						-17.688	22.596		36.33
	1397	CG						-17.235	22.345		38.65
20	1398	CD						-17.384			42.37
30	1399	CE			190	•		-17.183	20.632		50.39
	1400	NZ			190			-15.806	•		
	1401	С			190			-17.219			39.26
	1402	0 .			190			-16.115			39.95
25	1403	N			191			-18.337	23.777		40.10
35	1404	CA			191			-18.235	23.658		39.42
	1405	CB			191			-19.543	23.098		39.52
	1406	CG OD1			191			-20.721	24.060		44.32
	1407		ASP					-21.170	24.306		39.96
40	1408		ASP					-21.200		1.00	
1 U	1409 1410	С	ASP					-17.804		1.00	
	1411	<i>N</i>	ASP					-17.604	24.922		41.35
	1412	N CA	LEU					-17.632		1.00	
	7477	CA	LEU	¤	192		13.263	-17.218	27.294	1.00	34.43

	1413	СВ	LEU	J B	192		19.877	-18	3.258	28.397	1.00	26.76
	1414	CG	LEU	В	192		19.100	-19	.585	28.315	1.00	23.82
	1415	CD1	LEU	В	192		19.659	-20	.569	29.310	1.00	16.92
	1416	CD2	LEU	JВ	192		17.607	-19	.345	28.582	1.00	16.92
5	1417	С	LEU	В	192		20.024	-15	.826	27.761	1.00	34.24
	1418	0	LEU	В	192		19.508	-15	.310	28.748	1.00	38.50
	1419	N	ARG	В	193		20.957	-15	.221	27.029	1.00	30.50
	1420	CA	ARG	В	193		21.484	-13	.900	27.358	1.00	29.14
	1421	СВ	ARG	В	193		22.587	-13	.507	26.377	1.00	23.71
10	1422	CG	ARG	В	193		23.838	-14	.307	26.522	1.00	24.21
	1423	CD	ARG	В	193		24.862	-13	.896	25.494	1.00	20.84
	1424	NE	ARG	В	193		26.131	-14	.599	25.681	1.00	31.16
•	1425	CZ	ARG	В	193	. :	27.191	-14	.455	24.890	1.00	37.18
	1426	NH1	ARG	В	193	:	27.141	-13	.630	23.846	1.00	39.87
15	1427	NH2	ARG	В	193	;	28.303	-15	.131	25.147	1.00	37.17
	1428	С	ARG	В	193	:	20.483	-12	.756	27.415	1.00	28.97
	1429	0	ARG	В	193	. :	20.638	-11	.853	28.225	1.00	29.31
	1430	N	ASP	В	194		19.465	-12	.764	26.566	1.00	24.43
	1431	CA	ASP	В	194	. :	18.520	-11	.660	26.588	1.00	26.20
20	1432	CB	ASP	В	194	:	18.180	-11	.217	25.157	1.00	21.25
	1433	CG	ASP	В	194	:	19.413	-10	.763	24.361	1.00	25.14
	1434	OD1	ASP	В	194	2	20.357	-10	.207	24.973	1.00	16.92
	1435	OD2	ASP	В	194	:	19.427	-10	.948	23.119	1.00	30.59
	1436	. C	ASP	В	194	1	L7.241	-11	.990	27.344	1.00	24.70
25	1437	0	ASP	В	194	1	16.638	-13	.043	27.133	1.00	31.23
٠.	1438	N	PRO	В	195	1	6.811	-11	.088	28.242	1.00	19.04
	1439	CD	PRO	В	195	1	17.403	-9	.779	28.558	1.00	16.92
	1440	CA	PRO	В	195	1	15.593	-11	.299	29.024	1.00	22.28
	1441	CB	PRO	В	195	1	5.552	-10	.077	29.935	1.00	21.56
30	1442	CG	PRO	В	195	1	6.229	-9	.044	29.139	1.00	18.86
	1443	С	PRO	В	195	1	.4.392	-11	.371	28.110	1.00	24.96
	1444	0	PRO	В	195	1	4.345	-10	.680	27.101	1.00	30.51
	1445	N	ASP	В	196	1	.3.431	-12	.217	28.450	1.00	22.33
	1446	CA	ASP	В	196	1	.2.237	-12	.347	27.631	1.00	21.67
35	1447	CB	ASP	В	196	1	1.826	-13	.808	27.522	1.00	21.17
	1448	CG	ASP	В	196	1	2.875	-14	.636	26.849	1.00	35.32
	1449		ASP			1	3.781	-15	.133	27.550	1.00	31.80
	1450	OD2	ASP	В	196	1	2.808	-14	.767	25.609	1.00	44.56
	1451	С	ASP	В	196	1	1.116	-11	.525	28.225	1.00	22.00
40	1452	0	ASP			1	0.049	-11	.363	27.633	1.00	22.34
	1453	N			197	. 1	1.381	10.	.999	29.409	1.00	24.46
	1454	CA			197	1	0.423	-10	.174	30.104	1.00	22.14
	1455	CB	LEU	В	197	•	9.336	-11.	036	30.748	1.00	16.92

	1456	CG	LEU	В	197		8.462	-10.	340	31.797	1.00	16.92
	1457	CDI	LEU	В	197		7.828	-9.	106	31.228	1.00	18.26
	1458	CD2	LEU	В	197		7.396	-11.	274	32.273	1.00	23.97
	1459	С	LEU	В	197	1	1.163	-9.	394	31.163	1.00	24.32
5	1460	0	LEU	В	197	1	2.064	-9.	913	31.809	1.00	31.10
	1461	N	ILE	В	198	1	0.806	-8.	128	31.312	1.00	25.23
	1462	CA	ILE	В	198	1	1.419	-7.	301	32.327	1.00	23.49
	1463	СВ	ILE	В	198	1	2.252	-6.	163	31.728	1.00	16.92
	1464	CG2	LLE	В	198	1	2.760	-5.	255	32.837	1.00	16.92
. 10	1465	CG1	LLE	В	198	1	3.434	-6.	755	30.956	1.00	19.52
	1466	CD1	ILE	В	198	1	4.494	-5.	751	30.554	1.00	16.92
	1467	С	ILE	В	198	1	0.312	-6.	750	33.205	1.00	26.00
	1468	0	ILE	В	198	•	9.458	-5.	983	32.760	1.00	23.12
	1469	N	ILE	В	199	1	0.336	-7.	191	34.457	1.00	30.16
15	1470	CA	ILE	В	199		9.361	-6.	808	35.457	1.00	31.89
	1471	СВ	ILE	В	199		9.169	-7.	966	36.461	1.00	31.40
	1472	CG2	ILE	В	199	1	3.241	-7.	539	37.597	1.00	35.99
	1473	CG1	ILE	В	199	8	3.635	-9.	194	35.709	1.00	30.96
	1474	CD1	ILE	В	199	8	3.432	-10.	422	36.562	1.00	25.50
20	1475	С	ILE	В	199	9	9.797	-5.	547	36.196	1.00	30.27
	1476	0	ILE	В	199	10	.973	-5.3	382	36.511	1.00	30.43
	1477	N	ARG	В	200	8	3.843	-4.	657	36.450	1.00	29.84
	1478	CA	ARG	В	200		0.102	-3.4	413	37.167	1.00	34.70
	1479	CB	ARG	В	200	9	.192	-2.2	235	36.190	1.00	38.24
25	1480	CG	ARG	В	200	9	.649	-0.9	923	36.828	1.00	38.39
	1481	CD	ARG	В	200	13	.047	-1.0	036	37.439	1.00	41.65
	1482	NE	ARG	В	200	11	.489	0.1	171	38.148	1.00	34.53
	1483	CZ	ARG	В	200	11	.935	1.2	290	37.572	1.00	18.77
	1484	NH1	ARG	В	200	12	.014	1.3	399	36.252	1.00	16.92
30	1485	NH2	ARG	В	200	12	.314	2.3	307	38.326	1.00	18.24
	1486	С	ARG	В	200	7	.949	-3.2	211	38.145	1.00	35.76
	1487	0	ARG	В	200	6	.783	-3.2	252	37.756	1.00	33.19
	1488	N	THR	В	201	8	.277	-3.0	01	39.414	1.00	38.28
	1489	CA	THR	В	201	7	.262	-2.8	35	40.449	1.00	37.05
35	1490	CB	THR	В	201	7	.586	-3.7	22	41.664	1.00	16.92
	1491	OG1	THR	В	201	8	.943	-3.5	03	42.070	1.00	29.17
	1492	CG2	THR	В	201	7	.417	-5.1	74	41.315	1.00	19.67
	1493	С	THR	В	201	7	.102	-1.4	05	40.940	1.00	39.68
	1494	0	THR	В	201	7	.833	-0.5	09	40.522	1.00	41.56
40	1495	N	SER	В	202		.129	-1.2		41.826		41.87
	1496	CA	SER	В	202					42.426		39.34
	1497	CB	SER	В	202	7	.157	0.6	79	42.992	1.00	19.15
	1498	OG	SER	В	202	6	.945	1.9	80	43.512	1.00	39.12

	1499	С	SER	В	202		5.190	1.151	41.538	1.00	40.05
	1500	0	SER	В	202		4.920	2.262	41.995	1.00	47.17
	1501	N	GLY	В	203		4.922	0.811	40.281	1.00	38.45
	1502	CA	GLY	В	203		4.287	1.762	39.377	1.00	37.08
5	1503	С	GLY	В	203		5.271	2.563	38.534	1.00	35.70
	1504	0	GLY	В	203		4.886	3.461	37.787	1.00	37.31
	1505	N	GLU	В	204	٠	6.550	2.231			29.52
	1506	CA	GLU	В	204		7.586	2.917	37.908	1.00	28.07
	1507	СВ	GLU	. В	204		8.952	2.653	38.538	1.00	26.30
10	1508	· CG	GLU	В	204	•	9.236	3.482	39.779	1.00	48.79
	1509	CD	GLÜ	, B	204		8.973	4.961	39.556	1.00	50.97
	1510	OE1	GLU	В	204		7.849	5.419	39.869	1.00	42.50
	1511	OE2	GLU	В	204		, 9.877	5.663	39.055	1.00	50.61
	1512	С	GLU	В	204		7.616	2.477	36.462	1.00	29.34
15	1513	0	GLU	В	204		7.878	1.317	36.175	1.00	34.97
	1514	N	LEU	В	205		7.354	3.408	35.552	1.00	24.91
	1515	CA	LĘU	В	205	•	7.371	3.119	34.120	1.00	25.98
	1516	CB	LEU	В	205		6.104	3.666	33.470	1.00	25.92
	1517	CG	LEU	В	205		4.825	3.056	34.050	1.00	23.50
20	1518	CD1	LEU	В	205		3.610	3.785	33.547	1.00	16.92
	1519	CD2	LEU	В	205		4.753	1.600	33.668	1.00	30.67
	1520	С	LEU	В	205		8.607	3.733	33.472	1.00	28.56
	1521	0	LEU	В	205		8.526	4.382	32.441	1.00	29.61
	1522	,N			206	٠,	9.758	3.,533,	434.093	100	33.33
25	1523	CA	ARG				10.992		33.561	1.00	37.25
	1524	CB					11.776	4.826	34.645	1.00	42.74
	1525	CG			206		10.936	5.391	35,782	1.00	40.30
	1526	CD	ARG				11.792	6.156	36.799	1.00	44.32
20	1527	NE	ARG				12.921		37.312		65.13
30			ARG				13.705	5.748	38.324	1.00	69.76
	1529		ARG				13.483		38.937	1.00	76.09
	1530		ARG				14.714	4.974	38.727		74.71
	1531	С	ARG				11.815		33.106	1.00	42.39
25	1532	0	ARG				11.384		33.228		42.90
35	1533	N	LEU				13.005		32.592		44.87
	1534	CA	LEU				13.887	2.114	32.150		48.66
	1535	CB	LEU				14.442	2.437			63.61
	1536	CG	LEU				13.391	2.281	29.657		70.49
40	1537		LEU				13.973	2.698	28.321		76.92
40	1538		LEU				12.916	0.827	29.600		75.21
	1539	C	LEU				15.001	1.932	33.175		47.29
	1540	0	LEU				15.499	0.821	33.372		47.01
	1541	N	SER	В	208		15.373	3.027	33.833	1.00	42.15

	1542	CA	SER B 20	8 16.40	7 3.001	34.866	1.00	32.73
	1543	СВ	SER B 20	8 15.92	6 2.180	36.062	1.00	33.90
	1544	OG	SER B 20	8 14.58	8 2.494	36.396	1.00	24.12
	1545	С	SER B 20	8 17.75	2 2.451	34.404	1.00	28.39
5	1546	0	SER B 20	8 18.48	0 1.841	35.193	1.00	29.45
	1547	N	ASN B 20	9 18.07	1 2.652	33.128	1.00	26.85
	1548	CA	ASN B 20	9 19.34	8 2.212	32.561	1.00	27.50
	1549	СВ	ASN B 20	9 20.46	8 3.114	33.127	1.00	16.92
	1550		ASN B 20		6 2.862	32.494	1.00	22.61
10	1551	OD:	L ASN B 20	9 21.95	4 2.602	31.300	1.00	26.46
	1552		2 ASN B 20			33.303	1.00	20.95
	1553		ASN B 20			32.814	1.00	32.21
	1554	0	ASN B 20	9 20.80	0.317	32.892	1.00	34.11
	1555	N	PHE B 210		2 -0.074	32.915	1.00	,34.72
15	1556	CA	PHE B 210	0 18.754	1 -1.504	33.172	1.00	30.65
	1557	CB	PHE B 210	0 . 17.651	l -1.991	34.122	1.00	21.62
	1558	CG	PHE B 210	17.790	-3.433	34.537	1.00	28.42
	1559	CD1			-3.875	35.195	1.00	32.07
	1560		PHE B 210		-4.344	34.283	1.00	24.66
20	1561		PHE B 210			35.594	1.00	22.48
	1562		PHE B 210	16.884	-5.663	34.677	1.00	24.33
	1563	CZ	PHE B 210	•	-6.090	35.334	1.00	18.91
	1564	C	PHE B 210	2.0	-2.309	31.881	1.00	30.28
	1565	0	PHE B 210	17.778	-2.197	31.101	1.00	26.90
25	1566	N	LEU B 211		-3.117	31.673	1.00.	31.38
	1567	CA	LEU B 211		-3.959	30.484	1.00	30.02
	1568	СВ	LEU B 211		-5.253	30.661	1.00	19.94
	1569	CG	LEU B 211		-6.354	31.512	1.00	17.90
00	1570		LEU B 211		-7.623	31.409	1.00	17.79
30	1571	CD2	LEU B 211	21.132	-6.619	31.024	1.00	28.12
	1572	С	LEU B 211		-3.287	29.183	1.00	33.52
	1573	0	LEU B 211		-3.841	28.414	1.00	35.70
	1574	N	PRO B 212		-2.094	28.902	1.00	34.82
	1575	CD	PRO B 212		-1.502	29.547	1.00	34.05
35	1576	CA	PRO B 212		-1.359	27.684	1.00	31.21
	1577	CB	PRO B 212		-0.183	27.724	1.00	30.61
	1578	CG	-PRO B 212		-0.762	28.411	1.00	33.84
	1579	С	PRO B 212		-2.188	26.400	1.00	28.88
	1580	0	PRO B 212	18.862	-2.209	25.578	1.00 2	28.95
40	1581	N	TRP B 213	20.905	-2.878	26.241	1.00	32.89
	1582	CA	TRP B 213	21.151	-3.705	25.062	1.00	34.16
	1583	СВ	TRP B 213	22.653	-3.980	24.928	1.00 3	36.50
	1584	CG	TRP B 213	23.024	-4.885	23.779	1.00 4	10.25

	11 0 0010										
	1585	CD	2 TRE	P	213		23.654	-4.494	22.559	1.00	41.82
	1586	CE	2 TRE	P	213		23.825	-5.664	21.782	1.00	42.56
	1587	CE.	3 TRE	РВ	213		24.096	-3.266	22.043	1.00	36.15
	1588	CD	1 TRE	РВ	213		22.837	-6.241	23.695	1.00	34.48
5	1589	NE:	1 TRE	В	213		23.317	-6.713	22.500	1.00	35.36
	1590	CZ	2 TRE	В	213		24.421	-5.640	20.516	1.00	41.79
	1591	CZ.	3 TRE	В	213		24.687	-3.244	20.783	1.00	44.66
	1592	CH	2 TRF	В	213		24.845	-4.426	20.035	1.00	41.35
	1593	С	TRP	B	213		20.375	-5.034	25.026	1.00	31.31
10	1594	0	TRP	В	213		19.551	-5.252	24.140	1.00	28.47
	1595	N	GLN	В	214		20.644	-5.922	25.978	1.00	29.42
	1596	CA	GLN	В	214		19.975	-7.220	26.027	1.00	27.98
	1597	СВ	GLN	В	214		20.420	-7.989	27.277	1.00	29.16
	1598	CG	GLN	В	214		21.926	-8.184	27.438	1.00	30.26
15	1599	CD	GLN	В	214		22.631	-7.032	28.150	1.00	35.27
	1600	OE1	GLN	В	214		23.720	-7.208	28.699	1.00	35.10
	1601	NE2	GLN	В	214		22.021	-5.852	28.137	1.00	36.97
	1602	С	GLN	В	214		18.442	-7.114	26.018	1.00	26.22
	1603	0	GLN	В	214		17.747	-7.935	25.414	1.00	26.19
20	1604	N	GLY	В	215		17.918	-6.101	26.695	1.00	24.50
	1605	CA	GLY	В	215		16.480	-5.932	26.755	1.00	20.34
	1606	C	GLY	В	215		15.870	-5.269	25.536	1.00	20.33
	1607	0	GLY	В	215		14.680	-4.978	25.537	1.00	19.80
	1608	N	ALA	В	216		16.671	-5.045	24.495	1.00	16.97
25	1609	CA	ALA				16.207	-4.397	23.265	1.00	17.93
	1610	CB	ALA				17.162	-4.710	22.109	1.00	17.20
	1611	С	ALA				. 14.773	-4.758	22.875	1.00	20.59
	1612	0	ALA				13.970	-3.865	22.602	1.00	23.60
20	1613	N			217		14.437	-6.049	22.854		24.42
30	1614	CA	TYR				13.073	-6.462	22.494	1.00	18.63
	1615	CB	TYR				13.070	-7.402	21.282	1.00	16.92
	1616	CG			217	•	13.921	-6.990		1.00	16.92
	1617		TYR				15.315			1.00	16.92
25	1618		TYR				16.092			1.00	16.92
35	1619		TYR				13.328		18.901	1.00	16.92
	1620		TYR				14.098	-6.230	17.779		16.92
	1621	CZ	TYR				15.476		17.840	1.00	16.92
	1622	OH	TYR				•	-6.095	16.735		16.92
40	1623	C	TYR				12.326		23.629		16.92
40	1624	0	TYR					-7.982	23.380		16.92
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	1671	N	THR	В	223		3.729	-3.485	37.486	1.00	27.43
	1672	CA	THR	В	223		2.747	-3.695	38.529	1.00	29.24
	1673	CB	THR	В	223 [.]		. 2.922	-5.072	39.179	1.00	30.96
	1674	OG	1 THR	в:	223		1.913	-5.255	40.173		38.54
5	1675	CG.	2 THR	B, S	223		4.290				18.62
	1676	i c	THR	В 2	223		2.913	-2.643			31.84
	1677	0	THR	в 2	223	٠	3.992	-2.094			30.89
	1678	N	ASP	В 2	224		1.842				36.42
	1679	CA	ASP	. В 2	224		1.895				40.14
10	1680	СВ	ASP	В 2	224	,	0.494				41.56
	1681	CG	ASP	В 2	224			0.206			46.72
	1682	OD:	l ASP	В 2	224		-1.144		,		43.47
	1683	OD2	2 ASP	В 2	224		0.928	0.693			54.57
	1684	С	ASP	В 2	224		2.480	-1.939			40.48
15	1685	0	ASP	В 2	224		3.280	-1.285	43.341		42.72
	1686	N	THR	B 2	225		2.085	-3.163	43.002		37.47
	1687	CA	THŖ	B 2	25	,	2.566	-3.806			37.52
	1688	СВ	THR	В 2	25		2.344	-5.347			32.35
	1689	OG1	THR	В 2	25		2.884	-5.882			45.94
20	1690	CG2	THR	В 2	25		0.853	-5.686	44.282		27.82
	1691	С	THR	В 2	25		4.045	-3.520	44.459		36.64
	1692	0	THR	В 2	25 ·		4.853	-3.545	43.525		32.74
	1693	N	LEU	В 2	26		4.374	-3.221		·	40.20
	1694	CA	LEU	в 2	26	٠, ,	5.742	-2.934	46.126		
25	1695	CB	LEU				5.768	-2.291			
	1696	CG	LEÚ	B- 2	26	• •	5.116	-0.918	47.627	1.00	16.92
	1697		LEU				5.462	-0.129	46.383	1.00	20.23
	1698	CD2	LEU				3.612	-1.053	47.765	1.00	16.92
20	1699	С	LEU				6.536	-4.225	46.145	1.00	34.39
30	1700	0	LEU 1				6.008	-5.281	46.476	1.00	33.65
	1701	N	TRP 1				7.815	-4.129	45.807	1.00	27.74
	1702	CA	TRP 1				8.661	-5.302	45.736	1.00	26.44
	1703	CB	TRP 1				10.104	-4.903	45.490	1.00	16.92
25	1704	CG	TRP I		•		10.987	-6.092	45.465	1.00	16.92
35	1705		TRP I				10.954	-7.160	44.513	1.00	24.25
	1706		TRP I				11.975	-8.066	44.869	1.00	21.82
	1707		TRP F				10.167	-7.437	43.388	1.00	27.14
	1708		TRP F				11.990	-6.386	46.338	1.00	16.92
40	1709	•	TRP E				12.589	-7.570	45.989	1.00	18.37
40	1710		TRP E				12.231	-9.229	44.140	1.00	17.65
	1711		TRP E				10.422	-8.590	42.665	1.00	22.73
	1712		TRP E				11.447	-9.473	43.046	1.00	19.73
	1713	С	TRP E	22	7		8.613	-6.284	46.898	1.00	29.41

	1714	0	TRP E	227	8.38	7 -7.475	46.683	1.00	29.54
	1715	i N	PRO B	228	8.852	2 -5.817	48.140	1.00	34.10
,	1716	CE	PRO B	228	9.31	5 -4.485	48.571	1.00	32.12
	1717	CA	PRO B	228	8.81	-6.738	49.281	1.00	33.56
5	1718	CE	PRO B	228	9.023	L -5.818	50.469	1.00	30.46
	1719	CG	PRO B	228	9.943	3 -4.792	49.913	1.00	31.06
	1720	С	PRO B	228	7.511	L -7.501	49.359	1.00	36.50
	1721	0	PRO. B	228	7.412	-8.499	50.067	1.00	39.78
	1722	N	ASP B	229	6.513	3 -7.023	48.620	1.00	38.84
10	1723	CA	ASP B	229	5.195	-7.645	48.581	1.00	37.34
	1724	СВ	ASP B	229	4.107	-6.564	48.528	1.00	34.82
	1725	CG	ASP B	229	3.782	-5.992	49.888	1.00	34.97
	1726	OD	1 ASP B	229	3.018	-5.009	49.953	1.00	49.11
	1727	OD	2 ASP B	229	4.275	-6.527	50.897	1.00	48.81
15	1728	С	ASP B	229	5.042	-8.564	47.370	1.00	35.86
	1729	0	ASP B	229	3.979	-9.139	47.164	1.00	38.47
•	1730	N	PHE B	230	6.100	-8.703	46.575	1.00	31.52
	1731	CA			6.047	-9.533	45.371	1.00	29.58
••	1732	СВ	PHE B		7.152	-9.127	44.382	1.00	30.24
20	1733	CG	PHE B		6.750	-9.240	42.922	1.00	39.74
	1734		1 PHE B		5.791	-8.388	42.380	1.00	35.52
	1735		2 PHE B		7.357	-10.171	42.082	1.00	36.37
	. 1736		l PHE B		5.447	-8.456	41.021	1.00	28.22
25	1737		2 PHE B		7.021	-10.247	40.727	1.00	28.28
25 .	1738	CZ	PHE B		6.066		40.199	1.00	28.51
	1739	С	PHE B		6.168	-11.020	45.695	1.00	31.09
	1740	0	PHE B			-11.582	45.722	1.00	31.82
	1741	N	ASP B			-11.642		1.00	30.72
20	1742	CA	ASP B			-13.056		1.00	32.63
30	1743	СВ	ASP B			-13.288			
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	1745		ASP B			-12.730		1.00	51.61
	1746		ASP B			-12.247		1.00	31.99
25	1747	C	ASP B			-13.930		1.00	36.99
35	1748	0	ASP B			-13.432		1.00	37.67
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40	1752	CG	GLU B			-18.694		1.00 3	
40	1753	CD	GLU B			•	44.129	1.00 3	
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	1802	CG	2 ILE	В	239		4.62	-17.300	33.613	1.0	31.10
	1803	CG	1 ILE	В	239		6.089	5 -15.920	35.115	1.0	16.92
5	1804	CD	1 ILE	В	239		6.73	-17.180	35.625	1.0	28.23
	1805	С	ILE	В	239		3.004	-15.159	33.022	1.00	30.58
	1806	0	ILE	В	239	•	3.148	-15.532	31.863	1.00	27.47
	1807	N	LEU	В	240		1.815	-15.041	33.587	1.00	30.48
	1808	CA	LEU	В	240	•	0.620	-15.292	32.805	1.00	34.89
10	1809	СВ	LEU	В	240		-0.616	-15.333	33.701	1.00	48.13
	1810	CG	LEU	В	240		-0.916	-16.644	34.422	1.00	43.96
	1811	CD	1 LEU	В	240		-2.158	-16.473	35.263	1.00	40.59
	1812	CD	2 LEU	В	240		-1.123	-17.752	33.410	1.00	43.57
	1813	С	LEU	В	240		0.483	-14.161	31.789	1.00	31.63
15	1814	0	LEU	В	240		0.454	-14.392	30.581	1.00	33.47
	1815	N	ALA	В	241		0.417	-12.934	32.293	1.00	33.00
	1816	CA	ALA	В	241		0.283	-11.754	31:448	1.00	35.65
	1817	СВ	ALA	B	241		0.095	-10.510	32.314	1.00	36.36
	1818	С	ALA	В	241		1.488	-11.570	30.547	1.00	40.07
20	1819	0	ALA	В	241		1.686	-10.494	30.002	1.00	43.62
	1820	N	TYR	В	242		2.287	-12.617	30.390	1.00	46.16
	1821	CA	TYR	В	242		3.482	-12.539	29.560	1.00	49.44
	1822	СВ	TYR	В	242		4.282	-13.835	29.674	1.00	42.71
	1823	CG	TYR	В	242		5.537	-13.870	28.843	1.00	37.89
25	1824	CD1	TYR :	В	242 ,	٠.	6.327	-12.738	28.680	1.00	38.49
	1825		TYR I				7.499	-12.786	27.932	1.00	37.07
	1826		TYR 1				5.950	-15.051	28.242	1.00	33.74
	1827		TYR I				7.115	-15.115	27.501	1.00	31.74
20	1828		TYR I				7.885	-13.986	27.346	1.00	33.16
30	1829	ОН	TYR E					-14.074			
	1830	С	TYR F			•	3.153	-12.230	28.106	1.00	56.18
	1831	0	TYR E				2.797	-11.093	27.788	1.00	77.34
	1832	N	ASN E				3.270	-13.212	27.217	1.00	62.00
25	1833	CA	ASN E				2.970	-12.947	25.812	1.00	65.83
35	1834	СВ	ASN E				3.531	-14.053	24.911	1.00	65.24
	1835	CG	ASN E					-13.500	23.715	1.00	65.31
	1836		ASN E				5.303	-12.807	23.873	1.00	63.84
	1837		ASN B				3.831	-13.806	22.513	1.00	65.91
40	1838	С	ASN B				1.456	-12.828	25.643	1.00	69.21
40	1839	0	ASN B				0.694	-13.666	26.142	1.00	69.74
	1840	N	ARG B				1.033		24.957	1.00	68.62
	1841	CA	ARG B				-0.385	-11.484	24.723	1.00	71.05
	1842	CB	ARG B	2	44		-0.991	-10.800	25.955	1.00	71.10

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	1864	C12 E	PP (2	21.19	9 -7.990	47.403	1.00 74.41
•	1865	C13 F	PP C	2	21.55	4 -9.256	47.774	1.00 73.49
5	1866	C14 F	PP C	2	22.73	1 -10.024	47.224	1.00 74.43
	1867	C15 F	PP C	2	20.81	6 -10.087	48.804	1.00 73.47
	1868	PA F	PP C	2	13.814	1.633	46.280	1.00 96.03
	1869	O1A F	PP C	2	14.399	2.089	47.657	1.00 94.67
	1870	O2A F	PP C	2	13.930	2.601	45.086	1.00 95.64
. 10	1871	оза г	PP C	2	12.383	1.423	46.754	1.00 97.67
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	1874	O2B F	PP C	2	12.142	3.835	47.158	1.00103.25
	1875	O3B F	PP C	2	10.046	2.557	47.285	1.00101.13
15	1876	OH2 W	AT W	1	4.773	7.298	32.511	1.00 36.80
	1877	OH2 W	W TA	2	6.323	0.871	14.427	1.00 36.80
	1878	OH2 W	AT W	3	15.515	-0.599	23.674	1.00 36.80
	1879	OH2 W	W TA	4	-7.863	3.523	18.482	1.00 36.80
••	1880	OH2 W	W TA	5	16.858	9.374	28.786	1.00 36.80
20	1881	OH2 W		6	11.507	-3.595	14.868	1.00 36.80
	1882	OH2 W		7	34.098	13.685	24.109	1.00 36.80
	1883	OH2 W		8	-6.504	15.936	17.044	1.00 36.80
	. 1884	OH2 WA		9	16.680	15.674	27.816	1.00 36.80
25	1885	OH2 WA		10	16.423		25.423	1.00 36.80
25	1886	OH2 WA		11	-0.276	12.147	0.194	1.00 36.80
	1887	OH2 WA		12	41.369	13.097	17.334	1.00 36.80
	1888	OH2 WA		13	22.635	10.116	22.907	1.00 36.80
	1889	OH2 WA		14	15.672	1.557	26.009	1.00 36.80
30	1890	OH2 WA		15	19.186	15.106	27.885	1.00 36.80
30	1891	OH2 WA		16	39.396	4.075	29.930	1.00 36.80
	1892	OH2 WA		17		21.078		1.00 36.80
	1893 1894	OH2 WA		18	10.020		1.405	1.00 36.80
	1895	OH2 WA		19		-10.033	21.137	1.00 36.80
35	1896	OH2 WA		20	7.776	-6.623	10.879	1.00 36.80
33	1897	OH2 WA		. 21	19.914	-3.586	15.083	1.00 36.80
	1898	OH2 WA		22	-12.008	5.707	9.673	1.00 36.80
	1899	OH2 WA		23	8.883	29.025	9.092	1.00 36.80
	1900	OH2 WAS		24	24.894	18.337	19.301	1.00 36.80
40	1901	OH2 WAS		25 26	8.252	24.015	19.421	1.00 36.80
.0	1902	OH2 WAS		26 27		8.770	13.621	1.00 36.80
	1903	OH2 WAT		27		3.613	19.856	1.00 36.80
	1904	OH2 WAT		28	-1.747		-3.436	1.00 36.80
	7704	OHZ WAT	. ••	29	37.326	11.576	17.425	1.00 36.80

	1905	OH2	2 WAT	ŗ w	30		14.148	-10.191	16.523	1.00	36.80
	1906	OH	AW S	r w	31		15.836	20.107	8.725	1.00	36.80
	1907	OH	2 WAT	r w	32		4.798	11.641	14.018	1.00	36.80
	1908	OH2	AW S	r w	33		-7.822	7.982	31.296	1.00	36.80
5	1909	ОН2	AW S	. W	34		3.598	15.873	33.954	1.00	33.31
	1910	ОН2	CAW S	W	35		10.074	21.605	, 27.336	1.00	33.31
	1911	ОН2	CAW S	W	36	•	18.840	22.270	14.224	1.00	33.31
	1912	OH2	CAW S	W	37		-1.792	24.266	11.374	1.00	33.31
	1913	OH2	EAW S	· W	38	,	-8.931	8.878	19.966	1.00	33.31
10	1914	OH2	raw s	. M	39		-3.553	21.551	14.907	1.00	33.31
	1915	OH2	AW S	· W	4.0		8.399	-0.175	13.515	1.00	33.31
	1916	OH2	RAW	W	41		-6.204	12.470	11.990	1.00	33.31
	1917	OH2	KW S	W	42		4.589	8.276	34.603	1.00	33.31
	1918	ОН2	RAW	' W	43		28.648	16.280	19.235	1.00	33.31
15	1919	OH2	: WAI	W	44		18.590	15.236	-2.478	1.00	33.31
	1920	ОН2	: WAI	W	45		-9.057	0.909	19.891	1.00	33.31
	1921	OH2	raw :	W	46	•	-4.172	-4.775	22.498	1.00	33.31
	1922	ОН2	WAI	M	47		2.411	6.885	32.413	1.00	33.31
	1923	OH2	TAW	W	48		12.792	13.554	÷5.547	1.00	33.31
20	1924	OH2	TAW	M	49		-4.512	-6.634	11.993	1.00	33.31
	1925	OH2	WAT	W	50		-1.349	8.211	-3.909	1.00	33.31
	1926	OH2	WAT	W	51		13.234	14.853	39.074	1.00	33.31
	1927	OH2	WAT	M	52		37.819	4.036	7.107	1.00	33.31
	.1928	. OH2	WAT	W	5.3	٠.	-3.499	3.773	29.867	1.00	33.31
25	1929	OH2	WAT	W	54		2.292	20.765	40.034	1.00	33.31
	1930	OH2	WAT	W	55 '		15.806	-0.857	-1.454	1.00	33.31
	1931		WAT		56		3.305		15.620	1.00	36.80
	1876		TAW		1		3.683	-7.531	28.746	1.00	36.80
20	1877		WAT		2		16.001	-0.936			36.80
30	1878		,		3		17.436	0.631	29.046	1.00	36.80
	1879		WAT		4		2.416	-3.880	47.608	1.00	36.80
	1880		WAT		5			-9.355			36.80
	1881		WAT					3.621			36,80
25	1882		WAT				32.005	-13.312	17.093	1.00	36.80
35	1883		WAT	•				-16.254		1.00	36.80
	1884		WAT		9			-15.650		1.00	36.80
	1885		TAW		10			-23.017		1.00	36.80
	1886		WAT		11			-12.220		1.00	36.80
40		OH2			12		41.898	-12.537	17.893	1.00	36.80
40	1888		WAT		13			-9.945	25.171	1.00	36.80
	1889	OH2			14				27.107	1.00	36.80
		OH2			15			-15.036		1.00	36.80
	1891	OH2	WAT	X	16		32.358	-3.652	9.291	1.00	36.80

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1892 OH2 WAT X
                      17
                               22.480 -20.917
                                               22.300 1.00 36.80
            OH2 WAT X
      1893
                       18
                               26.786
                                        9.394 49.961
                                                       1.00 36.80
      1894
            OH2 WAT X
                       19
                               24.764 10.222
                                               26,384
                                                       1.00 36.80
      1895
            OH2 WAT X
                       '20
                               19.198
                                      6.611
                                               43.913
                                                       1.00 36.80
  5
      1896
            OH2 WAT X
                      . 21
                               26.159
                                       3.765
                                              33.066 1.00 36.80
      1897
           OH2 WAT X
                       22
                                4.678 -6.071 57.076
                                                     1.00 36.80
      1898
            OH2 WAT X
                       23
                               21.861 -28.995
                                               44.438
                                                       1.00 36.80
                               27.866 -18.095 26.551
      1899
            OH2 WAT X
                       24
                                                      1.00 36.80
      1900
           OH2 WAT X
                       25
                               14.858 -24.079 36.759 1.00 36.80
 10
     1901
           OH2 WAT X
                       26
                                4.325 -9.116
                                              52.350 1.00 36.80
     1902
           OH2 WAT X
                      27
                               43.966 -2.985
                                              12.943
                                                     1.00 36.80
     1903
           OH2 WAT X
                       28
                               20.854 -5.533 60.983
                                                      1.00 36.80
     1904
           OH2 WAT X
                       29
                               38.644 -11.092
                                              20.340
                                                      1.00 36.80
     1905
           OH2 WAT X
                      30 .
                               20.619 10.252 35.552
                                                      1.00.36.80
 15
     1906
           OH2 WAT X
                      31
                               27.367 -19.948 40.456 1.00 36.80
     1907
           OH2 WAT X
                      32 .
                               7.746 -11.905 49.162
                                                     1.00 36.80
     1908 OH2 WAT X
                     33
                              -5.421 -8.437 37.514
                                                      1.00 36.80
     1909
           OH2 WAT X
                      34
                               2.031 -16.137 28.299
                                                      1.00 33.31
     1910
           OH2 WAT X
                      35
                              11.326 -21.697
                                              29.436
                                                      1.00 33.31
20
     1911
           OH2 WAT X
                      36
                              26.349 -22.099 34.269
                                                      1.00 33.31
     1912
          OH2 WAT X
                      37
                              11.987 -24.451 49.302
                                                      1.00 33.31
     1913
           OH2 WAT X
                      38
                               0.761 -9.265 47.080
                                                     1.00 33.31
     1914
          OH2 WAT X
                      39
                               8.361 -21.797 47.640
                                                     1.00 33.31
     1915 OH2 WAT X
                      40
                              18.174
                                       0.155
                                             41.426
                                                     1.00 33.31
25
     1916 OH2 WAT X
                      41 .
                               7.919 -12.744
                                             51.620 1.00 33.31
     1917
           OH2 WAT X
                      42
                               2.259 -8.529
                                              27.215
                                                      1.00 33.31
     1918
           OH2 WAT X
                      43
                             30.809 -15.968
                                             24.283
                                                      1.00 33.31
     1919
           OH2 WAT X
                      44
                              36.386 -14.940
                                              47.555
                                                      1.00 33.31
     1920 OH2 WAT X
                      45
                               0.555 -1.299
                                              47.259
                                                      1.00 33.31
30
     1921 OH2 WAT X
                      46
                              2.656
                                     4.453
                                             42.213 . 1.00 33.31
     1922 OH2 WAT X
                      47
                               1.885 -7.161
                                             30.291
                                                     1.00 33.31
     1923
          OH2 WAT X
                      48
                              33.715 -13.341
                                             53.569
                                                     1.00 33.31
     1924
          OH2 WAT X
                      49
                              8.875
                                      6:387
                                             50.669
                                                     1.00 33.31
     1925
          OH2 WAT X
                      50
                              21.512 -8.272
                                             61.092
                                                     1.00 33.31
35
     1926
          OH2 WAT X
                      51
                              6.385 -14.980
                                             18.308
                                                     1.00 33.31
     1927 OH2 WAT X
                      52
                              45.290 -3.463
                                             28.162
                                                     1.00 33.31
    1928
          OH2 WAT X
                      53
                             -1.227 -4.138
                                             35.973
                                                     1.00 33.31
    1929
          OH2 WAT X
                     54
                             -2.672 -21.100
                                             24.317
                                                     1.00 33.31
    1930
          OH2 WAT X
                     55
                             33.258 1.090
                                             48.566
                                                     1.00 33.31
40
    1931
          OH2 WAT X
                     56
                             12.796
                                    4.108
                                             42.960
                                                     1.00 36.80
    END
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PCT/US02/38715

Table IC
Atomic coordinates of UPPS in complex with IPP

8 N GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.157 25.128 74.330 1.00 72.7 15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 11.372 24.915 70.222 1.00 74. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 26 CB ALA A 21 15.203 20.117 69.409 1.00 19. 27 C ALA A 21 15.203 20.117 69.409 1.00 19. 27 C ALA A 21 15.203 20.117 69.409 1.00 19. 27 C ALA A 21 15.400 19.644 70.409 1.00 19. 29 N HIS A 22 14.748 18.298 67.860 1.00 43. 33 CD2 HIS A 22 14.489 17.536 66.631 1.00 49. 31 CB HIS A 22 15.467 15.386 64.509 1.00 37. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 40. 33 CCG HIS A 22 15.467 15.386 64.509 1.00 40. 36. NE2 HIS A 22 16.225 14.551 63.725 1.00 40. 36. NE2 HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 49. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.00 1.00 49. 37 C HIS A 22 16.225 14.551 63.00 1.00 49. 37 C HIS A 22 16.225 14.551 63.00 1.00 49. 3		CR	YST1	5.5	. 42	28	118.168	175	.973 9	0.00 90.	00 90	.00
2 CG GLN A 18 8.344 25.155 76.710 1.00 83.7 3 CD GLN A 18 7.166 25.025 77.641 1.00 85.5 4 OE1 GLN A 18 6.296 24.165 77.449 1.00 88.6 10 5 NE2 GLN A 18 7.131 25.869 78.670 1.00 86.1 6 C GLN A 18 8.855 24.342 73.075 1.00 71.5 7 O GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.569 26.528 74.025 1.00 72.7 15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 11.372 24.915 70.222 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 10.592 21.131 70.132 1.00 45. 25 20 CB PRO A 20 11.437 19.951 69.912 1.00 45. 26 CB ALA A 21 13.864 19.875 69.912 1.00 63. 27 C PRO A 20 12.560 69.270 1.00 39. 28 O RRO A 20 12.560 69.270 1.00 39. 29 N HIS A 22 12.862 20.855 68.195 1.00 43. 30 CA HIS A 21 15.203 20.117 69.408 1.00 43. 31 CB HIS A 22 14.488 17.536 66.631 1.00 49. 32 CG HIS A 22 15.865 16.347 66.896 1.00 43. 33 CD HIS A 22 17.314 14.206 64.388 1.00 40. 34 CD HIS A 22 17.314 14.206 64.388 1.00 40. 35 CEI HIS A 22 17.314 14.206 64.388 1.00 40. 36 NEZ HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 17.314 14.206 64.388 1.00 40.	5	ATO	· MC	RES	IDU	<u>JE</u>		<u>x</u>	<u>Y</u> '	<u>Z</u>	<u>0çc</u>	<u>B</u>
3 CD GLN A 18 7.166 25.025 77.641 1.00 85.5 4 OE1 GLN A 18 6.296 24.165 77.449 1.00 88.6 10 5 NE2 GLN A 18 7.131 25.869 78.670 1.00 86.1 6 C GLN A 18 8.855 24.342 73.075 1.00 71.5 7 O GLN A 18 7.697 24.074 72.743 1.00 71.7 8 N GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.157 25.128 74.330 1.00 72.7 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 9.836 23.216 71.156 1.00 74. 13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 76. 15 C VAL A 19 11.372 24.915 70.222 1.00 76. 16 O VAL A 19 11.372 24.915 70.222 1.00 76. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 10.592 21.131 70.132 1.00 45. 19 CA PRO A 20 10.557 19.077 69.022 1.00 63. 25 CO CB PRO A 20 10.557 19.077 69.022 1.00 63. 26 CB ALA A 21 13.864 19.872 69.932 1.00 36. 27 C PRO A 20 12.790 20.266 69.270 1.00 39. 28 O ALA A 21 15.203 20.117 69.408 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 31 CB HIS A 22 14.748 18.298 67.860 1.00 43. 32 CG HIS A 22 14.898 17.536 66.631 1.00 49. 33 CG HIS A 22 15.867 15.547 65.676 1.00 38. 34 NDI HIS A 22 15.805 16.347 66.896 1.00 40. 35 CEI HIS A 22 17.799 14.792 65.570 1.00 38. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40.6 37 C HIS A 22 17.591 14.792 65.570 1.00 40.		1	СВ	GLN	A	18	7	.946	25.118	75.253	1.00	80.17
4		2	CĢ	GLN	A	18	8	.344	25.155	76.710	1.00	83.70
10 5 NE2 GLN A 18 7.131 25.869 78.670 1.00 86.1 6 C GLN A 18 8.855 24.342 73.075 1.00 71.5 7 O GLN A 18 7.697 24.074 72.743 1.00 71.7 8 N GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.569 26.528 74.025 1.00 72.7 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 11.372 24.915 70.222 1.00 76. 14 CG2 VAL A 19 10.822 22.055 71.076 1.00 74. 14 CG2 VAL A 19 10.822 22.055 71.076 1.00 74. 16 CO VAL A 19 11.372 24.915 70.222 1.00 74. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 11.437 19.951 69.912 1.00 42. 25 20 CB PRO A 20 12.790 20.266 69.270 1.00 39. 23 0 PRO A 20 12.862 20.855 68.195 1.00 63. 22 C PRO A 20 12.862 20.855 68.195 1.00 43. 30 25 CA ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 30 25 CA ALA A 21 15.430 19.423 68.067 1.00 43. 31 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 31 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 31 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 31 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 32 CG HIS A 22 14.748 18.298 67.860 1.00 60. 33. 35 30 CA HIS A 22 14.748 18.298 67.860 1.00 40. 33. 32 CG HIS A 22 14.748 18.298 67.860 1.00 40. 33. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 40. 33. 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 33. 36 NE2 HIS A 22 17.279 14.792 65.570 1.00 40. 33. 36 NE2 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 49. 35 CE1 HIS A 22 17.314 14.206 66.330 1.00 49. 35 CE1 HIS A 22 17.314 14.206 66.330 1.00 49. 35 CE1 HIS A 22 17.314 14.206 66.330 1.00 49. 35 CE1 HIS A 22 17.314 14.206 66.330 1.00 49. 35 CE1 HIS A 22 17.314 14.206 66.630 1.00 49. 35 CE1 HIS A 22 17.314 14.2		3	CD	GLN	A .	18	7	.166	25.025	77.641	1.00	85.97
6 C GLN A 18 8.855 24.342 73.075 1.00 71.5 7 O GLN A 18 7.697 24.074 72.743 1.00 71.7 8 N GLN A 18 9.569 26.528 74.025 1.00 72.7 15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 11.372 24.915 70.222 1.00 76. 14 CG2 VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 10.822 22.055 71.076 1.00 72. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.135 69.332 1.00 63. 19 CA PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.430 19.423 68.067 1.00 43. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 31 CB HIS A 22 14.748 18.298 67.860 1.00 50. 33 CA HIS A 22 14.898 17.536 66.631 1.00 40. 34 ND1 HIS A 22 15.805 16.347 66.896 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 49. 37 C HIS A 22 13.591 17.041 66.038 1.00 49. 38 O HIS A 22 13.591 17.041 66.038 1.00 49.		4	OE1	GLN	A	18	6	.296	24.165	77.449	1.00	88.60
7 O GLN A 18 7.697 24.074 72.743 1.00 71.7 8 N GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.157 25.128 74.330 1.00 72.7 15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 10.822 22.055 71.076 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 11.437 19.951 69.912 1.00 42. 25 20 CB PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.249 19.423 68.067 1.00 43. 31 CB HIS A 22 14.748 18.298 67.860 1.00 50. 32 CG HIS A 22 14.888 17.536 66.631 1.00 49. 33 CD2 HIS A 22 15.805 16.347 66.896 1.00 40. 34 ND1 HIS A 22 15.805 16.347 66.896 1.00 40. 35 CE1 HIS A 22 15.467 15.386 64.509 1.00 37.4 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 17.314 14.206 64.388 1.00 40.	10	5	NE2	GLN	A	18	7	.131	25.869	78.670	1.00	86.19
8 N GLN A 18 9.569 26.528 74.025 1.00 72.8 9 CA GLN A 18 9.157 25.128 74.330 1.00 72.8 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 10.081 24.140 69.983 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 11.372 24.915 70.222 1.00 74. 16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 10.552 21.115 69.233 1.00 63. 19 CA PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 29 N HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.467 15.386 64.509 1.00 37. 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37. 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37. 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40. 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 15.591 17.041 66.038 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.00 49. 37 C HIS A 22 15.929 16.204 66.630 1.0		6	С	GLN	A	18	8	.855	24.342	73.075	1.00	71.58
9 CA GLN A 18 9.157 25.128 74.330 1.00 72.7 15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 15.430 19.423 68.067 1.00 43. 35 30 CA HIS A 22 14.748 18.298 67.860 1.00 50. 31 CB HIS A 22 14.748 18.298 67.860 1.00 49. 32 CG HIS A 22 15.805 16.347 66.896 1.00 40. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37. 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37. 36 NE2 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 16.225 14.551 63.725 1.00 40. 38 O HIS A 22 16.255 14.551 63.725 1.00 40.		7	0	GLN	A	18	7	. 697	24.074	72.743	1.00	71.79
15 10 N VAL A 19 9.929 23.964 72.392 1.00 76. 11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 11.437 19.951 69.912 1.00 42. 25 20 CB PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 43. 30 25 CA ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 27 C ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 38 O ALA A 22 14.748 18.298 67.860 1.00 50. 31 CB HIS A 22 14.748 18.298 67.860 1.00 40. 32 CG HIS A 22 15.467 15.386 64.509 1.00 37.6 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 40. 35 CE1 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49.		8	N	GLN	A	18	. 9	.569	26.528	74.025	1.00	72.89
11 CA VAL A 19 9.836 23.216 71.156 1.00 74. 12 CB VAL A 19 10.081 24.140 69.983 1.00 77. 13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.805 16.347 66.896 1.00 40. 32 CG HIS A 22 15.467 15.386 64.509 1.00 38. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 40. 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49.		9	CA	GLN	A	18	9	.157	25.128	74.330	1.00	72.72
12 CB VAL A 19	15	10	N	VAL	A	19	•	9.929	23.96	4 72.392	1.00	76.37
13 CG1 VAL A 19 8.898 25.079 69.823 1.00 76. 14 CG2 VAL A 19 11.372 24.915 70.222 1.00 74. 20 15 C VAL A 19 10.822 22.055 71.076 1.00 72. 16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 15.203 20.117 69.408 1.00 43. 27 C ALA A 21 15.430 19.423 68.067 1.00 49. 28 O ALA A 21 15.430 19.423 68.067 1.00 49. 31 CB HIS A 22 14.748 18.298 67.860 1.00 40. 32 CG HIS A 22 15.805 16.347 65.676 1.00 38. 33 CD2 HIS A 22 15.805 16.347 65.676 1.00 38. 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37. 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49. 38 O HIS A 22 13.591 17.041 66.038 1.00 49.		11	CA	VAL	Α	19		9.836	23.21	6 71.156	1.00	74.76
14 CG2 VAL A 19		12	СВ	VAL	Α	19	. 1	0.081	24.14	0 69.983	1.00	77.30
20		13	CG1	. VAL	Α	19		8.898	25.07	9 69.823	1.00	76.99
16 O VAL A 19 11.780 21.982 71.841 1.00 73. 17 N PRO A 20 10.592 21.131 70.132 1.00 45. 18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 11.437 19.951 69.912 1.00 42. 25 20 CB PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 14.898 17.536 66.631 1.00 49. 32 CG HIS A 22 15.805 16.347 66.896 1.00 40. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.1 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49. 38 O HIS A 22 13.591 17.041 66.038 1.00 49.		14	CG2	VAL	Α	19	1	1.372	24.91	70.222	1.00	74.13
17 N PRO A 20	20	15	С	VAL	Α	19	1	0.822	22.05	5 71.076	1.00	72.83
18 CD PRO A 20 9.422 21.115 69.233 1.00 63. 19 CA PRO A 20 11.437 19.951 69.912 1.00 42. 25 20 CB PRO A 20 10.557 19.077 69.022 1.00 62. 21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.805 16.347 66.896 1.00 40. 32 CG HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37.8 35 NE2 HIS A 22 17.279 14.792 65.570 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49. 38 O HIS A 22 13.591 17.041 66.038 1.00 49.		16	0	VAL	A	19	1:	1.780	21.98	2 71.841	1.00	73.33
19 CA PRO A 20		17	N	PRO	A	20	10	0.592	21.13	1 70.132	1.00	45.38
25 20 CB PRO A 20			CD			20		9.422			1.00	63.68
21 CG PRO A 20 9.821 20.101 68.208 1.00 63. 22 C PRO A 20 12.790 20.266 69.270 1.00 39. 23 O PRO A 20 12.862 20.855 68.195 1.00 36. 24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.805 16.347 66.896 1.00 40. 32 CG HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40. 36 NE2 HIS A 22 17.314 14.206 64.388 1.00 40. 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	~ ~		CA			20	1:	1.437	19.95	69.912	1.00	42.31
22 C PRO A 20	25		CB	PRO	A	20	10	0.557	19.07	69.022	1.00	62.36
23 O PRO A 20							9	9.821	20.101	68.208	1.00	63.80
24 N ALA A 21 13.864 19.872 69.932 1.00 43. 30 25 CA ALA A 21 15.203 20.117 69.408 1.00 43. 26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.805 16.347 66.896 1.00 40. 32 CG HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.8 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.8 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.8 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.5							12	2.790	20.266	69.270	1.00	39.14
30 25 CA ALA A 21							12	2.862	,		1.00	36.95
26 CB ALA A 21 16.249 19.644 70.409 1.00 19. 27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49.3 31 CB HIS A 22 15.805 16.347 66.896 1.00 40.3 32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.6 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	20						13	3.864			1.00	43.53
27 C ALA A 21 15.430 19.423 68.067 1.00 43. 28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49. 31 CB HIS A 22 15.805 16.347 66.896 1.00 40. 32 CG HIS A 22 16.130 15.547 65.676 1.00 38. 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40. 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.0 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	30						15	5.203	20.117	69.408	1.00	43.37
28 O ALA A 21 16.207 19.899 67.238 1.00 41. 29 N HIS A 22 14.748 18.298 67.860 1.00 50. 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49.3 31 CB HIS A 22 15.805 16.347 66.896 1.00 40.3 32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.3 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3									19.644	70.409	1.00	19.22
29 N HIS A 22 14.748 18.298 67.860 1.00 50.3 35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49.3 31 CB HIS A 22 15.805 16.347 66.896 1.00 40.3 32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.3 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3									19.423			43.25
35 30 CA HIS A 22 14.898 17.536 66.631 1.00 49.3 31 CB HIS A 22 15.805 16.347 66.896 1.00 40.3 32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.3 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3											1.00	41.42
31 CB HIS A 22 15.805 16.347 66.896 1.00 40.3 32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.3 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.3 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	25										1.00	50.77
32 CG HIS A 22 16.130 15.547 65.676 1.00 38.3 33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.3 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.3 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	<i>33</i> .								•		1.00	49.24
33 CD2 HIS A 22 15.467 15.386 64.509 1.00 37.8 34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.9 40 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.0 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3										•		
34 ND1 HIS A 22 17.279 14.792 65.570 1.00 40.0 40 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.0 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.0 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3												•
40 35 CE1 HIS A 22 17.314 14.206 64.388 1.00 40.0 36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3											1.00	37.84
36 NE2 HIS A 22 16.225 14.551 63.725 1.00 40.3 37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	40										1.00	40.51
37 C HIS A 22 13.591 17.041 66.038 1.00 49.3 38 O HIS A 22 12.929 16.204 66.630 1.00 49.3	40										1.00	40.05
38 O HIS A 22 12.929 16.204 66.630 1.00 49.9												
00.030 1.00 45.0											1.00	49.35
			0	HIS	A	22	12	.929	16.204 319	66.630	1.00	49.93

	. 39	N	ILI	ΞΑ	23		13.229	17.556	64.865	1.00	50.60
	40	CA	IL	ΞΑ	23		12.012	17.127	64.185	1.00	52.08
	41	СВ	ILE	E A	23		11.116	18.303	63.770	1.00	52.30
	42	CG2	2 ILE	ΞA	23		9.907	17.785	63.017	1.00	49.04
5	43	CG	l ILE	ΞA	23		10.606	19.039	64.996	1.00	52.99
	44	CDI	LILE	C A	23	•	9.575	18.258	65.745	1.00	55.11
	45	С	ILE	E A	23		12.372	16.371	62.914	1.00	53.34
	46	0	ILE	E A	23		13.278	16.763	62.186	1.00	52.81
	47	N	GLY	A	24	'	11.664	15.280	62.655	1.00	55.59
10	48	CA	GLY	. A	24		11.916	14.510	61.454	1.00	55.68
	49	С	GLY	' A	24		10.636	14.558	60.652	1.00	57.28
	50	0	GLY	A	24		9.561	14.279	61.188	1.00	58.15
	51	N	ILE	: A	25		10.723	14.925	59.379	1.00	60.87
	52	CA	ILE	A	25		9.518	14.997	58.574	1.00	60.55
15	53	СВ	ILE	A	25	٠	9.274	16.407	58.016	1.00	44.36
	54	CG2	ILE	A	25		7.783	16.649	57.880	1.00	43.36
	55	CG1	ILE	A	25		9.863	17.464	58.946	1.00	43.88
	56	CD1	ILE	Α	25		9.805	18.870	58,385	1.00	40.84
	57	С	ILE	А	25		9.628	14.080	57.388	1.00	61.16
20	58	0	ILE	A	25		10.688	13.955 [.]	56.781	1.00	61.90
	59	N	ILE	Α	26		8.526	13.430	57.062	1.00	50.76
	60	CA	ILE	· A	26	•	8.491	12.557	55.912	1.00	51.38
	61	CB	ILE	A	.26		7.771	11.250	56.229	1.00	39.40
	62	CG2	ILE	A	26	*	7.530	10.469	54.944	1.00	36.96
25	63	CG1	ILE	·A	26		8.590	10.437	57.231	1.00	38.89
	64	CD1	ILE	A	26		7.963	9.106	57.576	1.00	36.95
	65	С	ILE	Α	26		7.669	13.332	54.905	1.00	52.89
	66	0	ILE	A	26		6.455	13.472	55.089	1.00	52.47
	67	N	MET	Ά	27		8.333	13.838	53.861	1.00	56.05
30	68	CA	MET	·A	27		7.696	14.642	52.808	1.00	57.51
	69	CB	MET	A	27		8.733	15.596	52.181	1.00	43.28
	70	CG	MET	A	27		9.433	16.489	53.193	1.00	37.98
	71	SD	MET	A	27		10.718	17.550	52,514	1.00	33.89
	72	CE	MET	A	27		12.040	16.489	52.414	1.00	32.98
35	73	С	MET	A	27		6.998	13.821	51.708	1.00	61.12
	74	0	MET		27		7.577	13.539	50.653	1.00	61.44
	75	N	ASP	A	28		5.738	13.469	51.968	1.00	78.26
	76	CA	ASP	A	28		4.906	12.680	51.056	1.00	81.87
40	77	CB	ASP		28		4.483	11.376	51.743	1.001	06.31
40	78	CG	ASP		28		3.741	10.431	50.809	1.001	08.55
	79		ASP		28		4.298	10.095	49.740	1.001	09.62
	80		ASP	A	28		2.609	10.016	51.146	1.001	09.84
	81	С	ASP	A	28		3.655	13.455	50.635	1.00	83.95

	82	0	ASP A	28	3.23		51.319	1.00 83.92
	83	·N	GLY A	29	3.05		49.515	1.00106.68
	84	CA	GLY A	29	1.86		49.020	1.00107.99
	85	С	GLY A	29	2.20	14.690	47.911	1.00109.08
5	86	0	GLY A	29	1.35	15.050	47.089	1.00110.54
	87	N	ASN A	30	3.46	7 15.109	47.906	1.00 49.18
	88	CA	ASN A	30	4.02	L 16.044	46.933	1.00 49.76
	89	CB	ASN A	30	5.550	15.954	47.000	1.00 59.70
	90	CG	ASN A	30	6.24	3 17.124	46.348	1.00 58.94
10	91	OD1	ASN A	30	7.40	17.402	46.641	1.00 57.39
	92	ND2	ASN A	30	5.546	5 17.811	45.452	1.00 60.12
	93	С	ASN A	30	3.505	15.720	45.525	1.00 51.86
	94	0	ASN A	30	3.456	16.575	44.637	1.00 51.26
	95	N	GLY A	31	3.121	14.469	45.322	1.00 95.59
15	96	CA	GLY A	31	2.597	14.087	44.033	1.00 98.36
	97	С	GLY A	31	1.105	14.334	44.044	1.00100.46
	98	0	GLY A	31	0.622	15.299	43.451	1.00100.95
•	99	N	ARG A	32	0.384	13.460	44.745	1.00100.88
	100	CA	ARG A	32	-1.06	8 13.529	44.859	1.00102.40
20	101	CB	ARG A	32	-1.52	4 12.829	46.138	1.00 88.53
	102	CG	ARG A	32	-2.96	2 12.357	46.121	1.00 88.65
	103	CD	ARG A	32	-3.28	9 11.704	47.441	1.00 89.95
	104	NE	ARG A	32	-3.12	8 12.661	48.534	1.00 92.42
	105	CZ	ARG A	32	-3.10	1 12.339	49.826	1.00 93.94
25	106	NH1	ARG A	32	-3.22	1 11.072	50.204	1.00 93.86
٠,	107	NH2	ARG A	32	-2.95	4 13.288	50.746	1.00 94.90
	108	С	ARG A	32	-1.53	6 14.972	44.871	1.00103.65
	109	0	ARG A	32	-2.62	1 15.288	44.375	1.00103.26
	110	N	TRP A	33	-0.71	0 15.845	45.439	1.00 95.39
30	111	CA	TRP A	33	-1.04	4 17.255	45.501	1.00 97.04
	112	CB	TRP A	33	-0.00	2 18.031	46.298	1.00 86.98
	113	CG	TRP A	33	-0.28	4 19.509	46.337	1.00 87.76
	114	CD2	TRP A	33	0.48	9 20.547	45.720	1.00 87.70
	115	CE2	TRP A	33	-0.14	4 21.772	46.017	1.00 87.59
35	116	CE3	TRP A	33 -	1.65	5 20.560	44.943	1.00 87.55
,	117	CD1	TRP A	33	-1.32	9 20.130	46.962	1.00 87.37
	118	NE1	TRP A	33	-1.25	0 21.489	46.774	1.00 87.39
	119	CZ2	TRP A	33	0.35	3 22.999	45.568	1.00 87.37
٠	120	CZ3	TRP A	33	2.14	5 21.780	44.497	1.00 86.53
40	121	CH2	TRP A	33	1.49	7 22.981	44.812	1.00 86.99
	122	С	TRP A	33	-1.12	9 17.841	44.104	1.00 98.03
	123	0	TRP A	33	-2.22	2 17.953	43.544	1.00 98.44
	124	N	ALA A	34	0.02	18.209	43.546	1.00103.06

•	125	CA	ALA	A	34		0.086	18.809	42.212	1.00103.60
	126	СВ	ALA	Α	34		1.553	19.001	41.778	1.00 43.07
	127	С	ALA	Α	34		-0.692	18.001	41.163	1.00104.15
	128	0	ALA	A	34		-0.767	18.388	39.998	1.00104.13
5	129	N	LYS	A	35		-1.278	16.884	41.585	1.00102.73
	130	CA	LYS	Α	35		-2.070	16.049	40.689	1.00104.36
	131	СВ	LYS	A	35		-2.305	14.670	41.327	1.00103.46
	132	CG	LYS	A	35		-2.952	13.616	40.416	1.00103.78
	133	CD	LYS	A	35		-4.481	13.720	40.345	1.00104.86
. 10	134	CE	LYS	A	35		-5.060	12.605	39.472	1.00104.77
	135	ΝZ	LYS	Α	35		-6.547	12.587	39.430	1.00103.24
	136	С	LYS	A	35		-3.409	16.750	40.409	1.00104.89
	137	0	LYS	A	35	•	-3.633	17.247	39.303	1.00104.89
	138	N	LYS	A	36		-4.283	16.799	41.415	1.00108.67
15	139	CA	ĻYS	A	36		-5.596	17.433	41.288	1.00108.81
	140	CB	LYS	A	36		-6.275	17.496	42.656	1.00116.28
	141	CG	LYS	A	36		-7.584	18.276	42.663	1.00116.03
	142	CD	LYS	A	36		-7.654	19.234	43.851	1.00115.08
	143	CE	LYS	A	36		-6.594	20.332	43.760	1.00114.82
20	144	NZ	LYS	A	36		-6.626	21.277	44.921	1.00113.37
	145	С	LYS	A	36		-5.547	18.844	40.694	1.00108.73
	146	0	LYS	A	36		-6.529	19.321	40.115	1.00108.16
	147	N	ARG	A	37		-4.407	19.510	40.850	1.00111.25
٥٢	148	CA	ARG		37		-4.226	20.863	40.334	1.00111.49
25	149	CB	ARG		37		-2.984	21.503	40.954	1.00 99.74
	150	CG	ARG		37		-3.031	21.668	42.457	1.00100.08
	151	CD	ARG		37		-4.044	22.718	42.877	1.00100.41
	152	NE	ARG		37		-3.537	23.542	43.974	1.00100.65
20	153	CZ	ARG .		37		-3.282	23.099	45.203	1.00100.42
30	154		ARG :		37		-3.489	21.825	45.522	1.00100.28
	155		ARG			•	-2.800	23.938	46.110	1.00100.50
	156	С	ARG I		37		-4.071	20.885	38.817	1.00111.43
	157	0	ARG I		37		-3.974	21.957	38.222	1.00111.99
25	158	N	MET A		38		-4.049	19.707	38.198	1.00 98.41
35	159	CA	MET A		38		-3.875	19.595	36.749	1.00 97.99
	160	CB	MET A		38		-4.941	20.407	36.004	1.00115.32
	161	CG	MET A		38		-6.343	19.822	36.074	1.00116.27
	162	SD	MET A		38		-6.439	18.168	35.357	1.00117.85
40	163	CE	MET A		38		-6.633	18.546	33.608	1.00116.66
40	164	C	MET A		38		-2.483	20.107	36.393	1.00 97.09
	165	0	MET A		38		-2.304	20.916	35.478	1.00 96.60
	166	N	GLN A		39		-1.499	19.623	37.137	1.00 91.07
	167	CA	GLN A	4	39		-0.117	20.021	36.928	1.00 90.66

	168	СВ	GL	ĄИ	39		0.318	20.955	38.059	1.00 92.12
	169	CG	GL	N A	39		-0.117	22.368	37.829	1.00 91.01
	170	CD	GL	N A	39		0.473	22.901	36.551	1.00 90.64
	171	OE:	l GLi	N A	39		1.638	23.305	36.511	1.00 90.38
5	172	NE2	GLI	N A	39		-0.317	22.877	35.484	1.00 89.76
	173	С	GLI	N A	39		0.848	18.836	36.821	1.00 90.86
	174	0	GLi	N A	39		0.525	17.710	37.221	1.00 90.62
	175	N	PRO	A C	40		2.045	19.076	36.262	1.00106.45
	176	CD	PRO	A C	40		2.499	20.328	35.630	1.00 72.93
10	177	CA	PRO	A C	40		3.051	18.026	36.109	1.00106.75
	178	СВ	PRO	A C	40		4.011	18.626	35.090	1.00 73.27
	179	CG	PRO	A	40		3.981	20.077	35.443	1.00 73.16
	180	С	PRO	A	40		3.737	17.709	37.434	1.00107.09
	181	0	PRO	A	40		3.962	18.599	38.258	1.00106.50
15	182	N	ARG	A	41		4.058	16.437	37.640	1.00100.27
	183	CA	ARG	5 A	41		4.725	16.024	38.862	1.00100.09
	184	CB	ARG	3 A	41	1	5.176	14.571	38.754	1.00110.99
	185	ĆG	ARG	A	41		4.096	13.631	38.289	1.00111.15
	186	CD	ARG	A	41		2.975	13.533	39.298	1.00111.80
20	187	NE	ARG	A	41		1.922	12.624	38.847	1.00112.39
	188	CZ	ARG	Α	41		2.111	11.345	38.524	1.00112.83
	189	NH1	ARG	A	41	i.	3.323	10.805	38.599	1.00112.44
	190	NH2	ARG	Α	41		1.083	10.601	38.130	1.00112.36
	191	С	ARG	Α	41 -	2000	5.940	16.921	39:069	1.00 99.99
25	192	0	ARG	A	41		6.215	17.356	40.185	1.00100.63
	193	N	VAL	A	42	•	6.659	17.206	37.986	1.00 93.73
	194	CA	VAL	Ä	42		7.847	18.048	38.072	1.00 93.74
	195	CB	VAL	A	42		8.355	18.480	36.684	1.00 99.03
	196	CG1	VAL	A	42		9.616	19.301	36.839	1.00 98.65
30	197	CG2	VAL	Α	42		8.631	17.265	35.821	1.00 99.84
	198	С	VAL	A	42		.7.527	19.298	38.869	1.00 93.42
	199	0	VAL	Α	42		8.127	19.553	39.908	1.00 93.37
	200	N	PHE	A	43		6.573	20.074	38.375	1.00110.29
	201	CA	PHE	Α	43		6.163	21.300	39.046	1.00110.29
35	202	CB	PHE	A	43		5.004	21.943	38.268	1.00136.60
	203	CG	PHE		43		4.281	23.027	39.021	1.00137.78
	204	CD1	PHE	A	43		4.967	24.130	39.519	1.00138.53
	205	CD2	PHE	A	43		2.904	22.940	39.233	1.00137.52
	206	CE1	PHE	A	43		4.293	25.131	40.219	1.00138.89
40	207	CE2	PHE	A	43		2.221	23.932	39.929	1.00137.63
	208	CZ	PHE	A	43		2.915	25.030	40.424	1.00138.21
	209	С	PHE	A	43		5.757	21.014	40.493	1.00109.11
	210	0	PHE	A	43		5.906	21.870	41.368	1.00108.34

,	211	N	GLY	A 4	4	5.250	19.806	40.735	1.00 84.30
	212	CA	GLY	A 4	4	4.834	19.423	42.076	1.00 83.06
	213	С	GLY	A 4	4	6.001	19.390	43.042	1.00 82.12
	214	0	GLY'	A 4	4	5.981	20.042	44.085	1.00 81.72
5	215	N	HIS.	A 4	5	7.025	18.619	42.698	1.00 92.58
	216	CA	HIS	A 4	5	8.207	18,530	43.539	1.00 92.23
	217	CB	HIS	A 4	5	9.121	17.388	43.057	1.00 89.47
	218	CG	HIS	A 4	5	8.646	16.023	43.467	1.00 89.70
	219	CD2	HIS	A 4	5 '	7.864	15.119	42.828	1.00 90.25
10	220	NDI	HIS	A 4	5	8.925	15.478	44.704	1.00 89.71
	221	CE1	HIS	A 4	5	8.334	14.300	44.808	1.00 89.80
	222	NE2	HIS	A 4!	5	7.683	14.059	43.684	1.00 90.18
	223	С	HIS	A 45	5	8.916	19.882	43.505	1.00 91.27
	224	0	HIS			9.828	20.149	44.296	1.00 91.42
15	225	N	LYS	•		8.487	20.734	42.577	1.00 82.42
	226	CA	LYS			9.034	22.081	42.465	1.00 81.87
	227	CB	LYS			8.683	22.710	41.114	1.00 97.17
	228	CG	LYS			9.491	22.162	39.947	1.00 99.47
00	229	CD	LYS			9.162	22.876	38.643	1.00 99.67
20	230	CE	LYS			10.094	22.419	37.536	1.00 99.93
	231	ΝZ	LYS			9.782	23.075	36.241	1.00100.68
	232	С	LYS			8.343	22.847	43.578	1.00 80.96
	233	O ::	LYS .			8.927	23.727	44.207	
25	234	N	ALA .			7.085	22.485	43.813	
25	235	CA	ALA		•	6.276	23.094	44.858	
	236	CB	ALA			4.819	23.105	44.452	1.00 69.13
	237	C	ALA A			6.466	22.241	46.094	1.00 75.37
	238 239	O N	ALA A			5.505	21.722	46.665	1.00 76.47
30	240	CA	GLY I			7.724	22.088	46.489	1.00 75.42
50	241	C	GLY A			8.044	21.284	47.651	1.00 74.30
	242	0	GLY A			9.323	21.784 21.985	48.278	1.00 74.36
	243	N	MET A			9.384 10.355	21.965	49.491	1.00 74.58
	244	CA	MET A			11.628	22.480	47.458	1.00 81.06
35	245	СВ	MET A			12.641	22.627	47.963 46.825	1.00 81.70
	246	CG	MET A			13.136	21.307	46.243	1.00 87.38
	247	SD	MET A			14.010	21.507	44.663	1.00 87.33
	248		MET A			12.610	21.420	43.554	1.00 87.62
	249		MET A			11.320	23.833	48.586	1.00 85.01
40	250		MET A			11.946	24.240	49.564	1.00 81.21
	251		GLU A			10.337	24.517	48.007	1.00 81.58
	252		GLU A			9.900	25.810	48.506	1.00 77.92 1.00 77.34
	253		GLU A			8.822	26.402	47.588	
				. 50		0.022	20.402	±1.500	1.00 95.37

										•	
	254	CG	GL	JA	50		9.050	27.860	47.157	1.00	95.61
	255	CD	GL	JA	50	,	9.139	28.834	48.326	1.00	96.16
	256	OE:	1 GL	JA	50		8.198	28.884	49.148	1.00	95.48
	257	OE:	2 GLU	JA	50		10.154	29.556	48.417	1.00	96.34
5	258	С	GL	JA	50		9.306	25.500	49.873	1.00	76.40
	259	0	GLU	JA	50		9.684	26.094	50.883	1.00	76.44
	260	N	ALA	A A	51		8.377	24.551	49.896	1.00	70.94
	261	CA	ALA	AA	51		7.741	24.135	51.142	1.00	69.92
	262	CB	ALA	A	51		6.856	22.914	50.889	1.00	99.69
10	263	С	ALA	Ā	51		8.798	23.817	52.207	1.00	68.95
•	264	0	ALA	A	51		8.601	24.073	53.393	1.00	68.42
	265	N	LEU	JA	52		9.914	23.242	51.775	1.00	66.05
	266	CA	LEU	JA	52		10.998	22.922	52.689	1.00	65.82
	267	СВ	LEU	A	52		12.066	22.062	51.993	1.00	68.86
15	268	CG	LEU	A	52		13.451	21.922	52.648	1.00	67.64
	269	CD1	LEU	Α	52		13.322	21.671	54.148	1.00	67.79
	270	CD2	LEU	Α	52		14.210	20.788	51.977	1.00	65.11
	271	С	LEU	Α	52		11.601	24.242	53.116	1.00	65.19
	272	0	LEU	Α	52 .		11.896	24.446	54.288	1.00	64.48
20	273	N	GLN	A	53		11.759	25.132	52.140	1.00	76.33
	274	CA	GLN	A	53		12.325	26.459	52.347	1.00	75.19
	275	CB	GLN	A	53		12.367	27.216	51.022	1.00	69.00
,	276	CG	GLN	Ą	53		13.340	28.356	51.018	1.00	68.46
	277	CD	GLN	A	53		14.740	27.863	51.257	1.00	68.74
25	278、	OE1	GLN	A	53		15.006	27.198	52.256	1.00	69.27
•	279	NE2	GLN	A	53		15.647	28.175	50.339	1.00	67.93
	280	С	GLN	A	53		11.519	27.265	53.355	1.00	74.92
	281	0	GLN	A	53		12.068	28.045	54.126	1.00	74.08
20	282	N	THR	A	54		10.209	27.081	53.334	1.00	84.09
30	283	CA	THR	A	54		9.340	27.782	54.258	1.00	84.86
	284	СВ	THR	A	54		7.870	27.659	53.820	1.00	67.41
	285		THR		54		7.669	28.444	52.639	1.00	68.01
	286		THR		54		6.922	28.124	54.928	1.00	66.49
2 5	287	С	THR		54		9.493	27.214	55.665	1.00	85.32
35	288	0	THR	A	54		9.546	27.970	56.638	1.00	86.21
	289	N	VAL	A	55		9.579	25.884	55.764	1.00	69.54
	290	CA	VAL		55		9.710	25.189	57.051	1.00	67.41
	291	CB	VAL		55		9.164	23.745	56.973	1.00	69.10
40	292		VAL		55		9.287	23.091	58.325	1.00	68.82
40	293		VAL		55		7.705	23.744	56.534	1.00	68.80
	294	С	VAL		55		11.128	25.141	57.625	1.00	67.02
	295	0	VAL		55		11.327	25.472	58.791	1.00	67.32
	296	N	THR	A	56		12.111	24.722	56.832	1.00	58.40

297 CA THR A 56 13.480 24.689 57.3	41 1.00 59.09
298 CB THR A 56 14.520 24.231 56.2	
299 OG1 THR A 56 15.859 24.425 56.75	
300 CG2 THR A 56 14.351 25.021 54.96	
5 301 C THR A 56 13.827 26.103 57.80	
302 O. THR A 56 14.827 26.327 58.50	
303 N LYS A 57 12.973 27.046 57.40	
304 CA LYS A 57 13.118 28.466 57.72	· · · · · · · · · · · · · · · · · · ·
305 CB LYS A 57 12.374 29.300 56.65	
10 306 CG LYS A 57 12.783 30.751 56.60	3 1.00 59.25
307 CD LYS A 57 12.913 31.221 55.15	88 1.00 60.46
308 CE LYS A 57 11.557 31.349 54.47	6 1.00 62.59
309 NZ LYS A 57 11.681 31.790 53.05	66 1.00 60.91
310 C LYS A 57 12.520 28.701 59.10	1.00 74.12
15 311 0 LYS A 57 13.228 29.020 60.06	2 1.00 74.74
312 N ALA A 58 11.204 28.526 59.17	1 1.00 63.23
313 CA ALA A 58 10.456 28.684 60.40	5 1.00 63.11
314 CB ALA A 58 9.019 28.284 60.18	2 1.00 34.72
315 C ALA A 58 11.089 27.785 61.45	2 1.00 63.84
20 316 O ALA A 58 11.256 28.172 62.61	2 1.00 63.83
317 N ALA A 59 11.434 26.575 61.02	8 1.00 82.06
318 CA ALA A 59 12.068 25.615 61.90	7 1.00 81.68
319 CB ALA A 59 12.589 24.453 61.10	0 1.00 82.06
320 C ALA A 59 13.219 26.302 62.63	
25 321 O ALA A 59 13.247 26.358 63.86	4 1.00 82.77
322 N ASN A 60 14.160 26.837 61.86	
323 CA ASN A 60 15.319 27.521 62.42	
324 CB ASN A 60 16.229 28.003 61.299 325 CG ASN A 60 17.591 28.441 61 789	•
20 000	
207 NDO PON P CO 10 110 27.750 02.05.	
200 0 200	
200	
220 %	
25 222 27 200	
331 CA LYS A 61 13.277 30.507 63.597 332 CB LYS A 61 12.132 31.127 62.786	
333 CG LYS A 61 11.459 32.356 63.412	
334 CD LYS A 61 10.527 33.060 62.407	
335 CE LYS A 61 9.436 32.130 61.884	
40 336 NZ LYS A 61 8.681 32.724 60.750	
200	
337 C LYS A 61 12.795 30.167 65.004	
337 C LYS A 61 12.795 30.167 65.004 338 O LYS A 61 13.407 30.563 65.993	1.00 63.12

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                                         29.024
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                                                          1.00 61.44
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            CB
                LEU A
                        62
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                                                  66.059
                                                           1.00 69.48
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                                8.665
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   5
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            CD2 LEU A
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                                         29.131
                                                 66.856
                                                          1.00 68.18
       345
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                                         27.423 67.997
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       349
            С
                GLY A
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                                14.637
                                         26.045
                                                 67.660
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                                15.771
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           CG1 VAL A
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 20
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           CG
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           CG1 VAL A
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      371
           CG2 VAL A
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                                                62.805
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               VAL A
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35
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               ILE A
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     377 'CG2 ILE A
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          CD1 ILE A
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          C
               ILE A
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                               16.686
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                                                        1.00 53.23
     382
          N
               THR A
                      68
                               15.117
                                       16.420
                                                60.304
                                                        1.00 48.41
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	383	CA	THR	A 68	15.480	15.449	59.294	1 00 47 12
	384				15.928			
	385				16.994			
	386				16.444			
5	387		THR	•	14.299			
	388				13.194			•
	389		VAL		14.560			
	390				13.575			
	391				13.657		55.062	
10	392		1 VAL	•	13.219		55.789	
	393		2 VAL		15.089			1.00 57.05
	394		VAL		13.773	•	55.190	1.00 38.18
	395		VAL 2		14.863		54.673	1.00 43.05
	396		TYR A		12.707	13.318	55.068	1.00 43.03
15	397		TYR A		12.760		54.325	1.00 62.67
	398	СВ	TYR A		11.929	11.009	55.031	1.00 52.64
	399	CG	TYR A		12.143	9.625	54.494	1.00 49.53
	400	CD	l TYR A	70	13.301	9.310	53.786	1.00 48.16
	401	CE I	L TYR A	70	13.526	8.026	53.316	1.00 47.14
20	402	CD2	TYR A	70	11.208	8.619	54.722	1.00 48.32
	403	CE2	YR A	70	11.424	7.329	54.260	1.00 48.99
	404	CZ	TYR A	70	12.587	7.041	53.557	1.00 48.59
	. 405	ОН	TYR A	. 70	12.816	5.770	53.100	1.00 48.72
•	406	С	TYR A	. 70	12.208	12.353	52.954	1.00 66.44
25	407	0	TYR A	70	11.023	12.625	52.796	1.00 65.91
	408	N	ALA A	71	13.077	12.270	51.959	1.00 68.56
	409	CA	ALA A	71	12.692	12.566	50.594	1.00 74.30
	410	CB	ALA A	71	13.886	13.176	49.878	1.00 72.73
20	411	С	ALA A	71	12.111	11.423	49.755	1.00 78.56
30	412	0	ALA A	71	12.851	10.771	49.016	1.00 78.80
	413	N	PHE A	72	10.796	11.197	49.859	1.00 83.41
	414	CA	PHE A	72	10.088	10.161	49.080	1.00 89.46
	415	CB	PHE A	72	11.012	8.973	48.765	1.00140.39
25	416	CG	PHE A	72	10.397	7.944	47.849	1.00144.03
35	417		PHE A	72	9.767	8.329	46.669	1.00145.48
	418		PHE A	72	10.457	6.588	48.163	1.00144.94
	419	CE1		72	9.204	7.378	45.815	1.00146.82
	420		PHE A	72	9.897	5.628	47.314	1.00146.70
40	421	CZ	PHE A	72	9.270	6.026	46.138	1.00147.70
40	422	C	PHE A	72	8.817	9.643	49.753	1.00 92.23
	423	0	PHE A	72	7.868	10.397	49.967	1.00 92.28
	424	N	SER A	73	8.809	8.343		1.00140.18
	425	CA	SER A	73	7.697	7.659	50.704	1.00143.09

	11 0 05/	04075								
	426	СВ	SER	A	73		7.333	8.400	51.987	1.00120.39
	427	OG	SER	A	73		8.499	8.670	52.748	1.00120.18
	. 428	Ç	SER	. A	73	•	6.448	7.467	49.837	1.00145.30
	429	0	SER	A	7,3		5.332	7.741	50.276	1.00145.74
5	430	N	THR	A	74		6.642	6.983	48.613	1.00161.50
	431	CA	THR	Α	74		5.544	6.735	47.677	1.00163.44
	432	СВ	THR	Α	74		4.495	5.764	48.297	1.00143.68
	433	OG1	THR	A	74		5.170	4.625	48.844	1.00143.22
	434	CG2	THR	Α	74		3.518	5.267	47:238	1.00143.83
10	435	С	THR	A	74		4.857	8.034	47.233	1:00164.62
	436	0	THR	A	74		5.346	9.129	47.523	1.00164.97
	437	N	GLU	A	75		3.738	7.887	46.520	1.00167.70
	438	CA	GLU	A	75	٠	2.920	8.983	45.978	1.00168.57
	439	CB	GLU	A	75		3.099	10.281	46.783	1.00113.85
15	440	CG	GLU	A	75 .		2.167	10.413	47.988	1.00112.90
	441	CD	GLU	Ά	75		0.722	10.670	47.599	1.00112.00
	442	OE1	GLU	A	75	·	-0.130	10.790	48.504	1.00110.81
	443	OE2	GLU	A	75		0.437	10.753	46.389	1.00111.35
	444	С	GLU		75		3.199	9.251	44.499	1.00169.23
20	445	0	GLU	A	75		2.777	10.272	43.953	1.00168.89
	446	N	ASN	A	76		3.909	8.331	43.853	1.00157.50
	447	CA	ASN	A	76		4.220	8.466	42.433	1.00158.07
	448	CB	ASN		76		5.667	8.052	42.148	1.00124.17
0.5	449		ASN			200	6.677	8.942	42.841	1.00123.19
25	450		ASN		76		6.695	10.157	42.643	1.00121.77
	451		ASN		76		7.528	8.339	43.657	1.00122.49
	452	С	ASN		76		3.265	7.577	41.651	1.00158.97
	453	0	ASN.		76		3.361	7.462	40.427	1.00159.05
20	454	N	TRP		77		2.348		42.380	1.00169.16
30	455	CA	TRP		77	•	1.347	6.066	41.791	1.00169.99
	456	СВ	TRP		77		0.583	6.809	40.693	1.00167.20
	457	CG	TRP		77		-0.286	7.902	41.215	1.00169.26
	458	CD2	TRP		77		0.095	9.260		1.00169.83
25	459	CE2			77		-1.030	9.928	41.965	1.00170.05
35	460	CE3			77		1.280	9.979	41.243	1.00169.57
	461		TRP		77.		-1.590	7.799	41.605	1.00169.57
	462	NE1	TRP		77		-2.045		42.057	1.00169.91
	463	CZ2	TRP		77		-1.005	11.282	42.301	1.00170.18
40	464	CZ3	TRP .		77		1.305	11.323	41.577	1.00169.40
40	465 466	CH2	TRP		77 77		0.169	11.961	42.099	1.00169.90
	466 467	C .	TRP		77 77		1.914	4.769	41.225	1.00169.29
	467	O N	TRP I		77 70		1.659		41.755	1.00169.41
	300	IN	THR I	M.	78		2.682	4.880	40.147	1.00115.73

	46	9 C.	А Т	HR :	A 78		3.248	3.70	39.51	9 1.00114.21
	47	0 C	в т	HR Z	A 78		2.400	3.26	38.30	3 1.00109.37
	47	1 0	31 T	HR Z	A 78		2.277	4.36	37.392	2 1.00108.51
	47	2 C	32 T	HR'	A 78	•	1.015	2.81	38.750	1.00109.06
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	47	5 N	A	RG A	A 79		5.142	2.922	38.268	1.00125.73
	47	6 C <i>I</i>	A Al	RG /	A 79		6.480	2.924	37.702	1.00124.36
	47	7 CE	B AI	RG I	¥ 79	•	6.630	4.068	36.696	1.00100.13
10	478	3 C	A A	RG I	4 79.		6.029	3.801	35.325	1.00 99.59
	479	e CE) AI	RG P	A 79		4.510	3.914	35.335	1.00 99.41
	480) NE	AF	RG A	79		3.943	3.589	34.028	1.00 99.30
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	490		PR	O. Y	80		9.135	-0.148	38.653	1.00 91.06
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	646	5 CD	2 TYR A	A 98 '		14.331	27.025	47.945	1.00 80.03
	647	7 CE	2 TYR F	98		13.020	27.176	47.501	1.00 80.71
	648	CZ	TYR A	98		12.577	26.440	46.420	1.00 81.85
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	651		TYR A	. 98		18.369	27.850	49.954	1.00 61.10
	652		VAL A			19.558	26.525	48.599	1.00 67.38
	653		VAL A			20.662	26.401	49.534	1.00 66.08
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	657		VAL A			21.348	27.747	49.802	1.00 65.56
	658	0	VAL A			21.954	27.943	50, 858	1.00 66.27
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	664	Ċ	PRO A			20.614		47.235	1.00 63.76
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	823	NZ	LYS A	120	30.845	14.418	35.807	1.00	73.90
	824	С	LYS A	120	26.995	13.389	40.063	1.00	74.96
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	828	СВ	GLN A	121	24.257	15.199	38.343	1.00	118.01
	829	CG	GLN A	121	23.363	16.432	38.550		119.87
	830	CD	GLN A	121	21.948	16.257	38.005	1.00	120.22
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20	832	NE2	GLN A	121	21.573	17.102	37.051	1.00	119.65
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	834	0	GLN A	121	25.486	16.384	41.314	1.00	95.10
	. 835	N	THR A	122	24.230	14.526	41.206	1.00	72.28
	836	CA	THR A	122	23.709	14.679	42.547		70.99
25	837	СВ	THR A	122	22.593	13.652	42.823	1.00	74.92
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25	846		PHE A		28.405		46.621	1.00	53.69
35			PHE A		30.046	12.518	45.014	1.00	55.49
			PHE A		29.387	11.766	47.588	1.00	54.44
			PHE A		31.038		45.973	1.00	54.03
			PHE A		30.710	12.056	47.263	1.00	54.36
40			PHE A			14.789	44.688	1.00	57.57
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	1220	CA	GLY	A 172	30.339	-7.450	75.145	1.00 66.18
	1221	С	GLY	A 172	30.734	-5.978	75.122	1.00 63.03
	1222	0	GLY	A 172	30.400	-5.209	76.029	1.00 62.01
	1223	N	ASP	A 173	31.461	-5.584	74.084	1.00 51.73
25	1224	CA	ASP	A 173	31.879	-4.202	73.942	1.00 49.09
٠.	1225	СВ	ASP	A 173	33.210	-4.146	73.194	1.00 94.86
	1226	CG	ASP .	A 173	33.742	-2.732	73.044	1.00 99.00
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	1228	OD2	ASP .	A 173	34.897	-2.494	73.461	1.00100.69
30	1229		ASP .	A 173	30.793	-3.461	73.157	1.00 45.66
	1230	0		A 173	30.590	-2.258	73.306	1.00 43.70
	1231	N	ILE	A 174	30.097	-4.197	72.306	1.00 66.57
	1232	CA	ILE	A 174	29.035	-3.618	71.516	1.00 63.27
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35	1234			A 174	27.359	-4.070	69.738	1.00 43.95
	1235			A 174	29.778	-4.548	69.333	1.00 46.82
	1236			A 174	29.596		68.244	1.00 47.02
	1237	С		A 174	27.829	-3.391	72.398	1.00 60.97
40	1238	0		A 174	27.384	-4.287	73.121	1.00 59.95
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	1289	ND2	ASN.	Α	181	29.560	5.566	70.106	1.00	43.29
5	1290	С	ASN	Α	181	28.021	5.583	65.565	1.00	47.23
	1291	0	ASN	A	181 .	28.492	6.332	64.714	1.00	48.29
	1292	N	TYR	A	182	27.658	4.340	65.286	1.00	43.54
	1293	CA	TYR	A	182	27.850	3.838	63.942	1.00	41.55
	1294	СВ	TYR	Ά	182	28.119	2.336	63.956	1.00	46.19
10	1295	CG	TYR	A	182	29.496	1.931	64.458	1.00	48.01
	1296	ÇD1	TYR	Ά	18,2	29.880	2.149	65.789	1.00	48.48
	1297	CE1	TYR	A	182	31.123	1.704	66.266	1.00	46.44
	1298	CD2	TYR	A·	182	30.398	1.263	63.616	1.00	47.00
	1299	CE2	TYR	A	182	31.641	0.816	64.088	1.00	46.87
15	1300	CZ	TYR	A	182 .	31.994	1.038	65.412	1.00	46.91
	1301	ОН	TYR	Ά	18.2	33.211	0.584	65.874	1.00	48.89
	1302	С	TYR	A	182	26.696	4.128	63.013	1.00	41.45
	1303	0	TYR	A	182	26.769	3.790	61.832	1.00	39.57
	1304	N	LEU	A	183	25.635	4.749	63.519	1.00	45.79
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	1306	CB	LEU	Α	183	23.218	5.203	63.490	1.00	39.84
	1307	CG	LEŬ	Α	183	22.754	3.944	64.233	1.00	36.79
	1308	CD1	LEU	A	183	21.519	4.267	65.018	1.00	36.60
	1309	CD2	LEU	A	183	22.457	2.828	63.260	1.00	36.31
25	1310	С	LEU	A	183	24.753	6.308	61.841	1.00	48.51
	1311	0	LEU	A	183	25.705	7.019	62.099	1.00	50.48
	1312	N	PHE	A	184	23.912	6.578	60.853	1.00	48.19
	1313	CA	PHE	A	184	24.091	7.747	59.994	1.00	49.49
	1314	СВ	PHE	A	184	23.081	7.725	58.849	1.00	44.20
30	1315	CG	PHE	A	184	23.347	6.671	57.820	1.00	44.57
	1316	CD1	PHE	A	184	22.477	6.497	56.760	1.00	44.44
	1317	CD2	PHE	A	184	24.448	5.837	57.922	1.00	44.74
	1318	CE1	PHE	A	184	22.696	5.506	55.821	1.00	44.26
	1319	CE2	PHE	A	184	24.676	4.841	56.988	1.00	43.37
35	1320	CZ	PHE	A	184	23.798		55.935	1.00	44.96
	1321	С	PHE	A	184	23.972	9.063	60.729	1.00	51.09
	1322	0	PHE	A	184	24.696	10.014	60.430	1.00	50.84
	1323	N	THR	A	185		9.115	61.678		46.98
		CA	THR	A	185		10.308	62.487		50.50
40	1325	CB	THR				10.113	63.422		44.57
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	1330	N	GLN	Α	186	25.079	9.799	63.323	1.00	56.18
	1331	CA	GLN	Α	186	26.291	9.988	64.115	1.00	60.77
	1332	СВ	GLN	Α	186	27.387	9.029	63.654	1.00	92.96
5	1333	CG	GLN	A	186	27.942	9.355	62.282	1.00	96.28
	1334	CD	GLN	A	186	29.106	8.469	61.894	1.00	98.93
	1335	OE1	GLN	A	186	28.952	7.260	61.722	1.00	100.11
	1336	NE2	GLN	.A	186	30.284	9.068	61.756	1.00	100.05
	1337	С	GLN	A	186	26.816	11.404	64.002	1.00	63.76
10	1338	0	GLN	A	186	27.168	12.022	65.005	1.00	64.46
	1339	N	HIS	A	187	26.867	11.905	62.769	1.00	63.31
	1340	CA	HIS	A	187 ·	27.360	13,246	62.470	1.00	64.48
•	1341	CB	HIS	Α	187	27.415	13.451	60.957	1.00	75.76
	1342	CG	HIS	A	187	28.288	12.465	60.246	1.00	76.39
15	1343	CD2	HIS	. A	187	28.006	11.552	59.286	1.00	77.37
	1344	ND1	HIS	Α	187	29.636	12.341	60.507	1.00	76.18
	1345	CE1	HIS	A	187	30.146	11.394	59.738	1.00	77.18
	1346	NE2	HIS	A	187	29.178	10.899	58.988 [.]	1.00	76.82
	1347	С	HIS	Α	187	26.502	14.333	63.091	1.00	65.00
20	1348	0	HIS	A	187	26.121	15.287	62.418	1.00	65.43
	1349	N	LEU	A	188	26.201	14.182	64.374	1.00	63.51
	1350	CA	LEU	A	188	25.383	15.142	65.101	1.00	64.86
	1351	,CB,	ΓĖΩ	A	188	23.888	14.904	64.818	1.00	67.36
	1352	CG	LEU	Α	188	23.177	15.455	63.567.	1.00	68.27
25	1353	CD1	LEU	A	188	23.581	14.720	62.288	1.00	67.48
	1354	CD2	LEU	A	188	21.674	15.303	63.785	1.00	68.32
	1355	С	LEU	A	188	25.649	15.042	66.607	1.00	66.30
	1356	0	LEU	A	188	26.180	14.047	67.097	1.00	66.36
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30	1358	CD	PRO	A	189	24.497	17.262	66.975	1.00	88.10
	1359	CA	PRO	A	189	25.505	16.047	68.810	1.001	00.81
	1360	CB	PRO	A	189	24.948	17.390	69.266	1.00	87.78
	1361	CG	PRO	A	189	23.841	17.634	68.273	1.00	88.99
	1362	С	PRO	A	189	24.804	14.869	69.480	1.001	00.89
35	1363	0	PRO	A	189	23.607	14.653	69.274	1.001	00.89
	1364	N	LYS	A	190	25.549	14.118	70.287	1.00	73.62
	1365	CA	LYS	A	190	24.995	12.961	70.983	1.00	73.72
	1366	CB	LYS	A	190	26.045	12.324	71.901	1.00	91.61
	1367	CG	LYS	A	190	27.125	11.528	71.183	1.00	95.52
40	1368	CD	LYS	A	190	27.938	10.688	72.165	1.00	96.56
	1369	CE	LYS	A	190	29.027	9.877	71.460	1.00	96.04
	1370	NZ	LYS	A	190	29.800	9.013	72.413	1.00	96.75
	1371	С	LYS	A	190	23.741	13.242	71.809	1.00	72.54

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	1375	СВ	ASP	A	191	22.312	15.829	73.526	1.00118.93
5	1376	CG	ASP	Α	191	23.039	17.042	72.955	1.00121.92
	1377	OD1	ASP	Α	191	24.050	16.861	72.242	1.00122.89
	1378	OD2	ASP	A	191	22.608	18.182	73.229	1.00122.16
	1379	С	ASP	A	191	20.831	15.253	71.584	1.00 80.20
	1380	0	ASP	A	191	19.785	15.671	72.084	1.00 79.39
10	1381	N	LEU	A	192	21.040	15.182	70.273	1.00 72.77
	1382	CA	LEU	A	192	20.038	15.597	69.294	1.00 69.38
	1383	СВ	LEU	A	192	20.429	16.939	68.684	1.00 72.72
	1384	CG	LEU	A	192	20.070	18.160	69.520	1.00 72.64
	1385	CD1	LEU	Α	192	21.228	19.131	69.548	1.00 74.95
15	1386	CD2	LEU	A	192	18.831	18.805	68.945	1.00 72.23
	1387	С	LEU	A	192	19.898	14.553	68.191	1.00 66.49
	1388	0	LEU	A	192	19.062	14.686	67.299	1.00 65.42
	1389	N	ARG	A	193	20.731	13.518	68.267	1.00 50.93
Ÿ	1390 -	CA	ARG	A	193	20.728	12.428	67.297	1.00 46.98
20	1391	СВ	ARG	A	193	21.658	11.312	67.794	1.00 49.52
	1392	CG	ARG	A	193	23.152	11.689	67.813	1.00 49.10
	1393	CD	ARG	A	193	24.032	10.612	68.489	1.00 47.28
	1394	NE	ARG	A	193	25.452	10.736	68.150	1.00 47.28
	1395	CZ	ARG	A	193	26.392	9.851	68.479	1.00 48.04
25	1396	NH1	ARG	A	193	26.082	8.759	69.170	1.00 46.77
·	1397	NH2	ARG	A	193	27.649	10.048	68.096	1.00 50.46
	1398	С	ARG	A	193	19.316	11.877	67.032	1.00 44.00
	1399	0	ARG	A	193	18.916	11.683	65.884	1.00 42.42
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	1402	CB	ASP	A	194	16.856	10.204	69.114	1.00 36.54
	1403	CG	ASP	A	194	17.866	9.102	69.308	1.00 34.55
	1404	OD1	ASP	A	194	18.675	8.865	68.376	1.00 34.00
		OD2	ASP	A	194	17.833	8.474	70.398	1.00 33.59
35	1406	С	ASP	A	194 .	16.093	12.181	67.840	1.00 32.88
	1407	0	ASP	A	194	15.891	12.988	68.742	1.00 31.68
	1408	N	PRO	A	195	15.341	12.163	66.739	1.00 34.77
	1409	CD	PRO	A	195	15.303	11.124	65.699	1.00 55.68
	1410	CA	PRO	A	195	14.260	13.130	66.563	1.00 34.35
40	1411	CB	PRO	A	195	13.481	12.560	65.388	1.00 55.61
	1412	CG	PRO	A	195	14.515	11.795	64.628	1.00 56.45
	1413	С	PRO	A	195	13.412	13.119	67.813	1.00 34.92
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	1415	N	ASP	A	196	12.916	14.277	68.226	1.00	38.18
	1416	CA	ASP	A	196	12.043	14.355	69.394	1.00	39.88
	1417	СВ	ASP	A	196	12.166	15.717	70.073	1.00	55.77
	1418	CG	ASP	Α	196	13.510	15.921	70.733	1.00	59.88
5	1419	OD1	ASP	· A	196	13.796	17.056	71.157	1.00	61,23
	1420	OD2	ASP	A	196	14.282	14.951	70.842	1.00	60.04
	1421	С	ASP	A	196	10.642	14.204	68.837	1.00	40.38
	1422	0	ASP	Α	196	9.694	13.901	69.555	1.00	40.86
	1423	N	LEU	A	197	10.529	14.414	67.528	1.00	58.18
10	1424	CA	LEU	A	197·	9.251	14.329	66.847	1.00	59.97
	1425	СВ	LEU	A	197	8.507	15.638	67.063	1.00	39.96
	1426	CG	LEU	A	197	7.114	15.766	66.476	1.00	38.32
	1427	CD1	LEU	Α	197	6.247	14.726	67.120	1.00	38.54
	1428	CD2	LEU	A	197	6.561	17.156	66.733	1.00	38.84
15	1429	С	LEU.	Α	197	9.378	14.031	65.346	1.00	61.27
	1430	0	LEŲ	Α	197	10.228	14.581	64.654	1.00	63.27
	1431	N	ILE	Α	198	8.513	13.152	64.859	1.00	51.40
	1432	CA	ILE	Α	198	8.478	12.748	63.456	1:00	51.63
	1433	СВ	ILE	A	198	8.564	11.212	63.339	1.00	32.05
20	1434	CG2	ILE	Α	198	8.183	10.775	61.968	1.00	29.63
*	1435	CG1	ILE	Α	198	9.982	10.743	63.666	1.00	31.32
	1436	CD1	ILE	Α	198	10.132	9.251	63.781	1.00	24.89
	1437	С	ΙĻΕ	A	198	7.150	13.219	62.870	1.00	54.08
	1438	0	ILE	A	198	6.130	13.140	63.545	1.00	55.97
25	1439	Ń	ILĖ	Α	199	7.149	13.709	61.629	1.00	55.58
	1440	CA	ILE	Α	199	5.903	14.182	61.011	1.00	57.03
	1441	СВ	ILE	A	199	5.928	15.712	60.782	1.00	61.40
	1442	CG2	ILE	Α	199	4.650	16.145	60.110	1.00	61.59
	1443	CG1	ILE	A	199	6.074	16.447	62.115	1.00	60.67
30	1444	CD1	ILE	A	199	6.203	17.943	61.985	1.00	57.19
	1445	С	ILE	A	199	5.585	13.509	59.674	1.00	58.15
	1446	0	ILE	A	199	6.399	13.520	58.748	1.00	59.57
	1447	N	ARG	A	200	4.394	12.925	59.586	1.00	40.62
	1448	CA	ARG	A	200	3.949	12.251	58.369	1.00	41.42
35	1449	СВ	ARG	Α	200	3.544	10.795	58.658	1.00	57.13
	1450	CG	ARG	A	200	3.372	9.936	57.402	1.00	54.89
	1451	CD	ARG	A	200	4.638	10.052	56.544	1.00	53.92
	1452	NE	ARG	A	200	4.596	9.341	55.268	1.00	52.83
	1453	CZ	ARG	A	200	4.486	8.024	55.138	1.00	51.74
40	1454	NH1	ARG	A	200	4.398	7.247	56.212	1.00	52.92
	1455	NH2	ARG	A	200	4.487	7.485	53.928	1.00	50.95
	1456	С	ARG	A	200	2.749	12.986	57.804	1.00	43.70
	1457	0	ARG	A	200	1.723	13.129	58.477	1.00	42.74

	1458	N	THR	A	201	2.877	13.448	56.565	1.00	71.25
	1459	CA	THR	A	201	1.798	14.174	55.908	1.00	74.12
	1460	СВ	THR	A	201	2.360	15.272	55.001	1.00	73.23
	1461	OG1	THR	A	201	2.913	14.673	53.828	1.00	76.28
5	1462	CG2	THR	Ά	201	3.459	16.038	55.711	1.00	74.06
	1463	С	THR	A	201	0.958	13.224	55.049	1.00	76.46
	1464	o	THR	A	201	1.174	12.011	55.048	1.00	78.25
	1465	N	SER	Α	202	-0.007	13.784	54.328	1.00	55.00
	1466	CA	SER	A	202	-0.872	13.006	53.448	1.00	54.41
10	1467	CB	SER	Ά	202	-0.103	12.603	52.196	1.00	53.35
•	1468	OG	SER	A	202	-0.890	11.747	51.391	1.00	52.76
	1469	C	SER	Α	202	-1.486	11.762	54.074	1.00	54.42
	1470	0	SER	A	202	-1.379	10.675	53.522	1.00	54.50
	1471	N	GLY	A	203	-2.131	11.934	55.224	1.00	69.79
15	1472	CA	GLY	A	203	-2.782	10.835	55.918	1.00	70.25
	1473	С	GLY	A	203	-2.218	9.446	55.678	1.00	71.00
	1474	0	GLY	A	203	-2.812	8.639	54.968	1.00	71.94
,	1475	N	GLU	A	204	-1.069	9.160	56.275	1.00	65.14
	1476	CA	GLU	A	204	-0.430	7.863	56.133	1.00	64.58
20	1477	СВ	GLU	A	204	0.783	7.975	55.207	1.00	89.40
	1478	CG	GLU	A	204	0.451	8.231	53.750	1.00	92.38
	1479	CD	GLU	A	204	0.034	6.970	53.018	1.00	94.85
	1480	OE1	GLU	A	204	-0.825	6.234	53.549	1.00	94.30
	1481	OE2	GLU	A	204	0.561	6.717	51.910	1.00	96.15
25	1482	C	GLU	A	204	0.025	7.430	57.516	1.00	63.86
٠,	1483	0	GLU	A	204	0.831	8.120	58.146	1.00	64.30
	1484	N	LEU	A	205	-0.485	6.300	57.998	1.00	77.27
	1485	CA	LEU	A	205	-0.083	5.810	59.312	1.00	75.81
	1486	CB	LEU	A	205	-1.307	5.355	60.110	1.00	73.73
30	1487	CG	LEU	A	205	-2.419	6.400	60.268	1.00	73.58
	1488	CD1	LEU	A	205	-3.189	6.111	61.540	1.00	72.43
	1489	CD2	LEU	A	205	-1.840	7.801	60.327	1.00	73.40
	1490	С	LEU	A	205	0.961	4.690	59.233	1.00	74.05
	1491	0	LEU	A	205	0.782	3.609	59.797	1.00	73.90
35	1492	N	ARG	A	206	2.046	4.978	58.516	1.00	44.09
	1493	CA	ARG	A	206	3.179	4.081	58.336	1,00	43.58
	1494	CB	ARG	A	20,6	3.292	3.601	56.888	1.00	79.95
	1495	CG	ARG	A	206	2.135		56.349	1.00	82.38
	1496	CD	ARG	A	206	2.503	2.233	54.984	1.00	86.62
40	1497	NE	ARG	A	206	1.323		54.148	1.00	90.07
	1498	CZ			206	0.615		53.615		91.34
	1499	NH1	ARG	A	206	0.973	4.292	53.824	1.00	90.96
	1500	NH2	ARG	A	206	-0.458	2.772	52.879	1.00	92.02

	1501	С	ARG A	206	4.	452	4.871	58.653	1.00	42.29
	1502	0	ARG A	206	4.	483	6.100	58.531	1.00	40.58
	1503	N	LEU A	207	5.	516	4.176	59.042	1.00	70.66
	1504	CA	LEU A	207	6.	755	4.889	59.327	1.00	68.57
5	1505	CB	LEU A	207	7.	466	4.298	60.552	1.00	67.93
	1506	CG	LEU A	207	8.	184	5.399	61.344	1.00	69.26
	1507	. CD	1 LEU A	207	7.	131	6.282	61.992	1.00	67.83
	1508	CD	2 LEU A	207	9.	114	4.820	62.390	1.00	69.87
	1509	С	LEU A	207	7.	683	4.883	58.100	1.00	66.21
. 10	1510	0	LEU A	207	8.	649	5.645	58.031	1.00	66.27
	1511	N	SER A	208	7.	384	4.017	57.138	1.00	48.52
	1512	CA	SER A	208	8.	152	3.937	55.895	1.00	44.95
	1513	CB	SER A	208	7.	897	5.193	55.061	1.00	49.44
	1514	OG	SER A	208	6.	505	5.438	54.934	1.00	53.00
15	1515	С	SER A	208	9.	655	3.741	56.049	1.00	42.59
	1516	0	SER A	208	10.	449	4.413	55.379	1.00	40.02
	1517	N	ASN A	209	10.	039	2.817	56.924	1.00	46.75
	1518	CA	ASN A	209 -	11.	446	2.513	57.161	1.00	45.16
	1519	CB	ASN A	209	11.	987	1.709	55.972	1.00	44.54
20	1520	CG	ASN A	209	13.	424	1.310	56.151	1.00	44.36
	1521	OD:	l ASN A	209	13.8	330	0.867	57.223	1.00	47.22
	1522	ND2	2 ASN A	209	14.2	208	1.459	55.101	1.00	45.74
	. 1523	С	ASN A	209	12.3	302	3.767	57.402	1.00	42.89
•	1524	0	ASN A	209	13.4	160	3.825	57.003	1.00	41.55
25 _.	1525	N	PHE A 2	210	11.7	725	4.756	58.079	1.00	39.22
	1526	CA	PHE A 2	210	12.3	399	6.024	58.365	1.00	37.27
	1527	CB	PHE A 2	210	11.4	157	7.183	58.032	1.00	38.93
	1528	CG	PHE A 2		12.0	01	8.538	58.390	1.00	38.93
	1529	CD1	PHE A 2	210	13.2	45	8.957	57.920	1.00	39.50
30	1530		PHE A 2		11.2	51	9.419	59.157	1.00	39.49
	1531		PHE A 2		13.7	24	10.234	58.211	1.00	36.40
	1532		PHE A 2		11.7	23	10.687	59.448	1.00	37.74
	1533	CZ	PHE A 2		12.9	57	11.092	58.973	1.00	37.09
~ ~	1534	С	PHE A 2	210	12.8	54	6.153	59.815	1.00	35.77
35	1535	0	PHE A 2		12.0	34	6.273	60.724	1.00	37.28
	1536	N	LEU A 2	11	14.1	65	6.135	60.024	1.00	30.72
	1537	CA	LEU A 2	11	14.7	40	6.266	61.356	1.00	29.17
	1538	CB	LEU A 2	11	14.5	62	7,710	61.849	1.00	30.75
4.6	1539	CG	LEU A 2		15.2	82	8.795	61.043	1.00	31.54
40	1540		LEU A 2		14.8			61.551	1.00	30.37
	1541		LEU A 2					61.149	1.00	29.89
	1542	С	LEU A 2	11	14.1	49	5.282	62.371	1.00	28.83
	1543	0	LEU A 2	11	13.7	27 .	5.666	63.461	1.00	30.11

	1544	N	PRO	A	212	14.144	3.989	62.038	1.00	21.34
•	1545	CD	PRO	A	212	14.827	3.341	60.910	1.00	25.09
	1546	CA	PRO	A	212	13.594	2.992	62.950	1.00	20.84
	1547	СВ	PRO	A	212	13.783	1.686	62.182	1.00	24.56
5	1548	CG	PRO	Ą	212	15.013	1.931	61.407	1.00	25.67
	1549	С	PRO	A	212	14.275	2.986	64.311	1.00	19.94
	1550	0	PRO	Α	212	13.606	2.967	65.341	1.00	17.23
	1551	N	TRP	A	213	15.607	3.016	64.308	1.00	28.93
	1552	CA	TRP	· A	213	16.364	3.005	65.550	1.00	28.92
10	1553	СВ	TRP	A	213	17.858	2.729	65.280	1.00	27.61
	1554	CG	TRP	Α	213	18.739	2.778	66.544	1.00	27.10
	.1555	CD2	TRP	A	213	19.294	1.661	67.264	1.00	27.80
	1556	CE2	TRP	A	213	19.977	2.186	68.395	1.00	25.65
	1557	CE3	TRP	A	213	19.277	0.271	67.071	1.00	27.47
15	1558	CD1	TRP	A	213.	19.106	3.896	67.253	1.00	25.51
	1559	NE1	TRP	A	213	19.843	3.547	68.362	1.00	25.34
	1560	CZ2	TRP	A	213	20.634	1.369	69.325	1.00	26.78
	1561	CZ3	ŤRP	A	213	19.927	-0.537	67.997	1.00	27.71
	1562	CH2	TRP	A	213	20.600	0.018	69.114	1.00	26.89
20	1563	С	TRP	A	213	16.206	4.322	66.307	1.00	29.52
	1564	0	TRP	A	213	15.844	4.325	67.479	1.00	30.08
	1565	N	GLN	A	214	16.461	5.436	65.626	1.00	25.53
	1566	CA	GLN	A	214	16.397	6.752	66.244	1.00	27.09
	1567	CB	GLN	A	214	16.892	7.820	65.265	1.00	32.69
25	1568	CG	GLN	A	214	18.366	7.748	64.882	1.00	31.73
	1569	CD	GLN	A	214	18.632	6.807	63.743	1.00	33.51
	1570	OE1	GLN	A	214	19.768	6.664	63.304	1.00	31.73
	1571	NE2	GLN	A	214	17.588	6.148	63.254	1.00	35.57
	1572	С	GLN	A	214	15.039	7.176	66.763	1.00	29.77
30	1573	0	GLN	A	214	14.952	7.775	67.830	1.00	30.98
	1574	N			215	13.979	6.872	66.012	1.00	31.51
	1575	CA	GLY	A	215	12.636	7.283	66.414	1.00	29.71
	1576	С	GLY	A	215	11.951	6.363	67.397	1.00	30,52
	1577	0	GLY	A	215	10.723	6.406	67.593	1.00	30.83
35	1578	N	ALA.	Α	216	12.769	5.536	68.032	1.00	27.55
	1579	CA	ALA	A	216	12.288	4.564	68.982	1.00	26.70
	1580	CB	ALA	A	216	13.457		69.675	1.00	23.13
	1581	С	ALA	A	216	11.335	5.186	69.980	1.00	27.72
40	1582	0	ALA			10.348	4.574	70.351	1.00	28.13
40	1583	N	TYR	A	217	11.608	6.407	70.417	1.00	31.29
	1584	CA			217	10.696	7.033	71.369	1.00	33.23
,	1585	CB	TYR			11.362	7.203	72.725	1.00	36.13
	1586	CG	TYR	A	217	11.285	5.961	73.584	1.00	36.90

	1587	CD1	TYR	217	12	.329	5.033	73.619	1.00	35.40
	1588	CE1	TYR P	217	12	.241	3.899	74.421	1.00	39.13
	1589	CD2	TYR A	217	10	.153	5.717	74.366	1.00	38.96
	1590	CE2	TYR	217	10	.052	4.593	75.165	1.00	38.12
5	1591	CZ	TYR A	217	11	.093	3.687	75 ⁻ .197	1.00	40.37
	1592	ОН	TYR F	217	. 10	.976	2.595	76.032	1.00	39.19
	1593	С	TYR A	217	10	.155	8.356	70.914	1.00	32.99
	1594	0	TYR F	217	9	.539	9.073	71.687	1.00	34.63
	1595	N	SER A	218	10	.375	8.659	69.643	1.00	29.75
10	1596	CA	SER A	218	9	.933	9.904	69.054	1.00	32.78
	1597	CB	SER A	218	10	.368	9.977	67.592	1.00	51.24
	1598	OG	SER A	218	11	.777	9, 986	67.465	1.00	56.29
	1599	С	SER A	218	8	.429	10.009	69.123	1.00	34.88
	1600	0	SER A	218	7.7	.734	9.020	68.899	1.00	,35.86
15	1601	N	GLU A	219	7	. 927	11.199	69.453	1.00	50.24
	1602	CA	GĻU A	219	. 6	.487	11.431	69.495	1.00	51.43
	1603	· CB	GLU A	219	6	.170	12.752	70.184	1.00	42.72
	1604	CG	GLU A	219	6	.133	12.682	71.698		42.50
	1605	CD	GLU A		4	.957	11.880	72.219	1.00	44.60
20	1606	OE1	GLU A	219	3	.985	11.711	71.458	1.00	45.34
	1607	OE2	GLU A			.992	11.430	73.386	1.00	45.20
	1608	С	GLU A				11.485	68.031		52.41
	1609	0	GLU A	n		.756	12.076	67.206	1.00	52.72
25	1610	N	LEU A			.958	10.861	,		39.96
25	1611	CA		220			10.819	1.		40.25
	1612	СВ	LEU A				9.395			26.28
	1613	CG	LEU A			132		66.411		19.24
	1614		LEU A			691		66.044		19.92
20	1615		LEU A			427	8.699	65.703		15.40
30	1616	С	LEU A			404	11.806	66.040		44.14
	1617	0	LEU A		2.			66.891		
	1618	N	TYR A			402	12.358			53.92
	1619	CA	TYR A			366	13.304	64.443		57.45
35	1620	CB	TYR A			864	14.740			63.62
33	1621 1622	CG CD1	TYRA			885	15.812			66.26
	1623		TYR A			565	15.809	64.647		66.77
	1624		TYR A			323	16.776	64.233		66.77
			TYR A			282	16.824	63.339		67.06
40	1625 1626		TYR A			400	17.788			67.52
70	1627	CZ OH	TYR A			106	17.758	63.373		67.28
	1628	C	TYR A			765	18.716	62.938		69.40
	1629	0	TYR A			924		62,990		58.86
	1023	J	TYR A	221	2.	717	13.187	62.048	T.00	59.20

	1630	N	PHE	A	222	0.649	12.741	62.821	1.00	60.95
	1631	CA	PHE	A	222	0.089	12.490	61.503	1.00	62.79
	1632	CB	PHE	A	222	-0.612	11.134	61.521	1.00	58.23.
	1633	CG	PHE	Α	222	0.307	9.989	61.848	1.00	58.94
5	1634	CDI	L PHE	Α	222	0.060	9.167	62.945	1.00	58.55
	1635	CD2	PHE	A	222	1.438	9.743	61.071	1.00	58.48
	1636	CE1	PHE	A	222	0.923	8.123	63.265	1.00	58.44
	1637	CE2	PHE	A	222	2.303	8.704	61.384	1.00	56.86
	1638	CZ	PHE	A.	222	2.043	7.893	62.486	1.00	58.47
10	1639	С	PHE	A :	222	-0.879	13.600	61.066	1.00	64.53
•	1640	0	PHE	A :	222	-1.436	14.312	61.897	1.00	65.86
	1641	N	THR	A :	223	-1.073	13.749	59.761	1.00	53.11
	1642	CA	THR	A :	223	-1.965	14.774	59.236	1.00	55.50
	1643	CB	THR	A :	223	-1.342	16.165	59.311	1.00	74.89
15	1644	OG1	THR	A :	223	-2.132	17.070	58.527	1.00	76.56
	1645	CG2	THR	A :	223	0.091	16.146	58.765	1.00	75.02
	1646	С	THR	A 2	223	-2.299	14.542	57.778	1.00	56.91
	1647	0	THR	A 2	223	-1.409	14.522	56.926	1.00	57.65
	1648	N	ASP	A 2	224	-3.588	14.414	57.486	1.00	75.10
20	1649	CA	ASP	A 2	224	-4.050	14.176	56.124	1.00	75.82
	1650	СВ	ASP	A 2	224	-5.566	14.070	56.114	1.00	72.96
	1651	CG	ASP	A 2	224	-6.087	13.245	57.269	1.00	74.62
	1652	OD1	ASP	A 2	224	-6.195	13.791	58.389	1.00	76.73
	1653	OD2	ASP .	A 2	224	-6.374	12.045	57.066	1.00	74.53
25	1654	С	ASP .	A 2	224	-3.599	15.245	55.138	1.00	76.24
•	1655	0	ASP .	A 2	224	-3.628	15.034	53.927	1.00	77.12
	1656	N	THR .	A 2	225	-3.168	16.387	55.655	1.00	47.98
	1657	CA	THR			-2.719	17.478	54.807	1.00	49.10
20	1658	CB	THR I			-2.165	18.619	55.655	1.00	84.57
30	1659	OG1	THR I			-1.082	18.129	56.453	1.00	86.07
	1660		THR I			-3.245			1.00	85.13
	1661	С	THR,			-1.636	17.020		1.00	48.17
	1662	0	THR Z			-0.790	16.225	54.216	1.00	49.64
	1663	N	LEU A			-1.674	17.506	52.615	1.00	51.52
35	1664	CA	LEU Z			-0.657	17.143	51.636	1.00	52.64
	1665	CB	LEU A			-1.046	17.626	50.237	1.00	72.33
	1666	CG	LEU A			-1.979	16.711	49.441	1.00	72.59
	1667		LEU A			-1.197	15.499		1.00	73.13
10	1668		LEU. A			-3.171	16.290		1.00	71.25
40	1669	С	LEU A			0.616	17.825	52.097		53.19
	1670	0	LEU A					53.081		53.08
	1671	N	TRP A				17.610	51.388		66.66
	1672	CA	TRP F	A 2	27	3.005	18.185	51.797	1.00	67.22

	1673	CB T	RP A	227	4	4.169	17.289	51.35	8 1.00	0 60.56
	1674	CG TE	RP A	227	į	5.518	17.915	51.60		58.17
	1675	CD2 TE	RP A	227	į	5.999	18.478	52.83	7 1.00	57.18
	1676	CE2 TF	RP A	227	-	7.291	18.995	52.58		57.49
5	1677	CE3 TF	P A	227	5	.466	18.598	54.12		56.47
	1678	CD1 TF	PA	227	6	5.514	18.105	50.688		58.25
	1679	NE1 TR	P A	227	7	7.579	18.753	51.26	5 1.00	58.32
	1680	CZ2 TR	P A	227	8	.056	19.624	53.573	3 1.00	56.36
	1681	CZ3 TR	PΑ	227	6	.232	19.226	55.113	1.00	55.66
. 10	1682	CH2 TR	P A	227	7	.511	19.729	54.826	1.00	55.52
	1683	C TR	PA:	227	3	.311	19.618	51.392	1.00	68.58
	1684	O TR	P A 2	227	3	.833	20.385	52.195	1.00	68.87
	1685	N PR	O A 2	228	3	.034	19.999	50.142	1.00	87.77
	1686		A C		2	.724	19.233	48.927	1.00	98.49
15	1687	•		228	3	.349	21.391	49.810	1.00	88.87
	1688) A 2		3	.046	21.462	48.318	1.00	99.05
	1689) A 2			.378	20.082	47.858	1.00	99.11
	1690	C PRO) A 2	228	2	.468	22.325	50.637	1.00	88.93
00	1691) A 2		2	.716	23.530	50.717	1.00	88.53
20	1692		P A 2			.448	21.736	51.260	1.00	95.84
			A 2			.490	22.450	52.105	1.00	95.31
			A 2		-0.	.862	21.732	52.076	1.00	72.45
			A 2		-1.	597	21.940	50.779	1.00	72, 47
25		OD1 ASF				571	21.198	50.517	1.00	73.15
25		OD2 ASP			-1.	201	22.856	50.030	1.00	72.04
			A 2			941	22.593	53.563	1.00	95.53
			A 2			234	23.193	54.384	1.00	95.46
			A 2			103	22.033	53.889	1.00	72.23
30			A 2			616	22.122	55.246	1.00	
50			A 23			607		55.533	1.00	60.91
				30		646	20.566	56.982	1.00	58.00
		CD1 PHE				548	19.941	57.566	1.00	•
		CD2 PHE				756	20.848	57.774	1.00	57.16
35		CE1 PHE				550	19.611	58.911	1.00	
0.5			A 23				20.523	59.119	1.00	
	1709 C		A 23				19.904	59.687	1.00 !	
	1710 C		A 23				23.473	55.349	1.00	
	1711 N		A 23				23.662	54.837	1.00 6	
40			A 23				24.407	56.008	1.0010	
			A 23		3.0		25.778	56.202	1.0010	
			A 23		1.9		26.755	55.898	1.00 6	
		D1 ASP			-0.3			56.683	1.00 6	
	. = -		23	-	-0.3	174	27.100	56.448	1.00 6	6.14

	1716	00	2 ASP A 231	0.696	25.531	57.534	1.00 63.85
	1717	C	ASP A 231	3.592	26.022	57.617	1.00106.25
	1718	0	ASP A 231	3.441	25.169	58.493	1.00105.19
	1719	N	GLU A 232	4.198	27.185	57.837	1.00 75.85
5	1720	CA	GLU A 232	4.689	27.513		
	1721	СВ	GLU A 232	5.089	28.981		
	1722	CG	GLU A 232		•		
	1723	CD	GLU A 232	6.249	30.743		
•	1724	OE	1 GLU A 232	6.592	31.336	59.605	
10	1725	OE	2 GLU A 232	6.284	31.276		•
	1726	С	GLU A 232	3.535	27.246		
	1727	0	GLU A 232	3.719	26.713	61.213	
	1728	N	ALA A 233	2.338	27:617	59.679	
	1729	CA	ALA A 233	1.132	27.406	60.472	
15	1730	СВ	ALA A 233	-0.110	27.612	59.608	
	1731	С	ALA A 233	1.164	25.980	60.987	1.00 67.42
	1732	0	ALA A 233	1.145	25.733		1.00 66.72
	1733	N	ALA A 234	1.223	25.049	60.040	1.00105.33
	1734	CA	ALA A 234	1.263	23.627	60.332	1.00104.96
20	1735	CB	ALA A 234	1.372	22.840	59.036	1.00 70.15
	1736	С	ALA A 234	2.447	23.318	61.229	1.00104.98
	1737	0	ALA A 234	2.283	22.770	62.317	
	1738	N	LEU A 235	3.639	23.676	60.768	1.00 81.94
	1739	CA	LEU A 235	. 4.843	23.427	61.536	1.00 81.18
25	1740	CB	LEU A 235	5.962	24.363	61.087	1.00 60.77
	1741	CG	LEU A 235	7.367	24.051	61.602	1.00 59.54
	1742		LEU A 235	7.388	24.143	63.099	1.00 59.47
	1743		LEU A 235	7.784	22.668	61.169	1.00 59.88
20	1744	С	LEU A 235	4.549	23.653	63.005	1.00 82.00
30	1745	0	LEU A 235	4.577	22.720	63.809	1.00 82.42
	1746	N	GLN A 236	4.258	24.901	63.351	1.00 79.63
	1747	CA	GLN A 236	3.968	25.252	64.735	1.00 79.41
	1748	CB	GLN A 236	3.717	26.758	64.864	1.00 86.03
25	1749	CG	GLN A 236	4.727	27.619	64.115	1.00 87.53
35	1750	CD	GLN A 236	4.724	29.069	64.564	1.00 88.57
	1751		GLN A 236	5.310	29.932	63.913	1.00 88.30
	1752		GLN A 236	· ·	29.339	65.688	1.00 90.39
	1753	C	GLN A 236			65.203	1.00 78.24
40	1754	0	GLN A 236	2.694		66.339	1.00 78.33
40	1755	N	GLU A 237				1.00 75.22
	1756	CA	GLU A 237	0.551		64.625	1.00 74.35
	1757	CB	GLU A 237			63.362	1.00 83.36
	1758	CG	GLU A 237	-1.792	23.489	63.582	1.00 85.49

	1759	CI	GLU A	237	-2.290	22.464	64.592	2 1.00	86.68
	1760	OE	1 GLU A	237	-1.986	22.616	65.796	1.00	87.49
	1761	OE	2 GLU A	237	-2.989	21.506	64.181	. 1.00	86.25
	1762	С	GLU A	237	0.945	22.269	65.199	1.00	73.31
5	1763	0	GLU A	237	0.373	21.810	66.189		72.96
	1764	N.	ALA A	238	1.937	21.636	64.580		68.54
	1765	CA	ALA A	238	2.418	20.337	65.043	1.00	67.12
	1766	СВ	ALA A	238	3.490	19.794	64.096	1.00	47.92
	1767	С	ALA A	238	3.001	20.507	66.440	1.00	65.44
10	1768	0	ALA A	238	2.659	19.769	67.368	1.00	64.92
	1769	N	ILE A	239	3.878	21.493	66.590	1.00	55.00
	1770	CA	ILE A	239	4.489	21.727	67.881	1.00	54.40
	1771	СВ	ILE A	239	5.429	22.917	67.829	1.00	40.35
	1772	CG:	2 ILE A	239	6.326	22.929	69.059	1.00	39.90
15	1773	CG:	l ILE A	239	6.297	22.805	66.587	1.00	37.77
	1774	CD:	l ILE A	239	7.497	23.715	66.621	1.00	39.44
	1775	С	ILE A	239	3.426	21.939	68.955	1.00	56.09
	1776	0	ILE A	239	3.558	21.442	70.072	1.00	55.65
20	1777	. N	LEU A 2		2.363	22.663	68.624	1.00	65.76
20	1778	CA	LEU A 2		1.312	22.871	69.606	1.00	67.84
	1779	CB	LEU A 2		0.124	23.614	68.990	1.00	93.15
	1780	CG	LEU A 2		-1.019	24.084	69.907	1.00	93.89
	. 1781		LEU A 2		-2.066	24.781	69.047	1.00	94,06
٥٢	1782		LEU A 2		-1.659	22.920	70.662	1.00	92.97
25	1783	С	LEU A 2		0.885	21.473	70.035	1.00	68.53
	1784	0	LEU A 2		0.593	21.226	71.205	1.00	68.37
	1785	N	ALA A 2		0.865	20.553	69.080	1.00	78.77
	1786	CA	ALA A 2		0.475	19.185	69.373	1.00	81.17
30	1787	CB	ALA A 2		0.189	18.439	68.082		73.59
30	1788	C	ALA A 2			18.464	70.171	1.00	82.11
	1789	0	ALA A 2		1.288	17.894	71.228	1.00	81.41
	1790	N Gr	TYR A 2		2.789	18.496	69.665	1.00	68.88
	1791	CA	TYR A 2		3.914	17.838	70.329	1.00	69.93
35	1792	CB	TYR A 2		5.236		69.789	1.00	
<i>33</i> ,		CG	TYR A 2		6.402	18.047	70.678	1.00	61.34
			TYR A 2		6.937	16.767	70.719	1.00	61.47
			TYR A 24		8.002	16.465	71.565	1.00	60.57
			TYR A 24		6.957	19.023	71.505	1.00	
40			TYR A 24		8.015	18.733	72.350	1.00 5	59.45
10		CZ	TYR A 24		8.530	17.454	72.375	1.00 5	
		OH C	TYR A 24				73.212	1.00 5	
			TYR A 24				71.831	1.00 7	
	TOOT	J	TYR A 24	2	4.059	17.097	72.603	1.00 7	2.12

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	1847	NE	ARG A 247	3.758	6.592	80.920	1.00 96.92
	1848	CZ	ARG A 247	2.638	5.878	80.794	1.00 97.32
5	1849	· NH	1 ARG A 247	1.540	6.452	80.313	1.00 97.34
	1850	NH	2 ARG A 247	2.615	4.592	81.139	
	1851	С	ARG A 247	7.688	9.168	78.571	1.00 79.63
	1852	0	ARG, A 247	7.713	8.084	79.165	
	1853	N	ARG A 248	8.567	9.512	77.629	1.00154.67
10	1854	CA	ARG A 248	9.652	8.645	77.165	1.00153,82
	1855	СВ	ARG A 248	10.791	9.474	76.559	1.00115.47
	1856	CG	ARG A 248	10.540	9,967	75.143	1.00115.68
	1857	CD	ARG A 248	11.821	10.526	74.520	1.00116.07
	1858	NE	ARG A 248	11.612	11.027	73.160	1.00117.85
15	1859	CZ	ARG A 248	12.588	11.430	72.348	1.00118.27
	1860	NHI	L ARG A 248	13.856	11.394	72.748	1.00118.12
÷	1861	NH2	2 ARG A 248	12.294	11.873	71.134	1.00117.73
	1862	С	ARG A 248	10.256	7.722	78.204	1.00153.01
	1863	0	ARG A 248	10.017	7.861	79.399	1.00152.98
20	1864	N	PHE A 249	11.058	6.779	77.720	1.00104.87
	1865	CA	PHE A 249	11.735	5.811	78.574	1.00104.55
	1866	СВ	PHE A 249	12.807	6.523	79.422	1.00 82.94
	1867	CG	PHE A 249	14.025	5.679	.,79716	1.00 82.52
	1868	CD1	PHE A 249	13.993	4.687	80.695	1.00 82.75
25	1869	CD2	PHE A 249	15.206	5.865	78.993	1.00 81.44
	1870	CE1	PHE A 249	15.124	3.891	80.950	1.00 81.36
	1871	CE2	PHE A 249	16.334	5.076	79.241	1.00 80.65
	1872	CZ	PHE A 249	16.290	4.089	80.221	1.00 79.85
•	1873	С	PHE A 249	10.708	5.148	79.481	1.00104.71
30	1874	0	PHE A 249	11.071	4.514	80.473	1.00105.55
	1875	N	GLY A 250	9.428	5.288	79.133	1.00 72.46
	1876	CA	GLY A 250	8.385		79.965	1.00 72.36
	1877	С	GLY A 250	8.435			1.00 72.32
25	1878	0	GLY A 250		6.669		1.00 71.99
35	1879	N	GLY A 251		4.667	82.397	1.00 72.26
	1880	CA	GLY A 251	8.620	5.270	83.720	1.00 71.88
	1881	С	GLY A 251	7.308		84.253	1.00 71.75
	1882	0	GLY A 251		5.882	83.523	1.00 71.62
40	1883	N	VAL A 252	7.292		85.529	1.00 71.62
40	1884	CA	VAL A 252			86.149	1.00 70.92
	1885	CB	VAL A 252	6.124		87.709	1.00 70.44
	1886		VAL A 252	4.700		88.293	1.00 68.98
	1887	CG2	VAL A 252	6.814	5.309	88.138	1.00 69.75

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	2277	С	ILE	В	67	1.11	7 -11.388	68.358	1.00	29.05
	2278	0	ILE	В,	67	1.38	2 -12.344	69.110	1.00	25.41
5	2279	N	THR	В	68	1.82	2 -10.253	68.344	1.00	36,80
	2280	CA	THR	В	68	2.93	1 -10.006	69.256	1.00	33.90
	2281	СВ	THR	В	68	4.22	6 -9.635	68.485	1.00	29.12
	2282	OG1	THR	В	68	4.68	4 -10.781	67.751	1.00	30.17
	2283	CG2	THR	В	68	5.31	9 -9.192	69:441	1.00	27.04
10	2284	С	THR	В	68	2.50	5 -8.875	70.164	1.00	33.51
	2285	0	THR	В	68	2.22	5 -7.758	69.710	1.00	30.56
	2286	N	VAL	В	69	2.43	6 -9.184	71.455	1.00	26.40
	2287	CA	VAL	В	69	2.00	8 -8.204	72.454	1.00	28.99
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15	2289	CG1	VAL	·B	69	-0.38	9 -8.722	72.899	1.00	36.17
	2290	CG2	VAL	В	69	1.41	3 -10.247	73.761	1.00	37.07
	2291	C	VAL	В	69	3.12	5 -7.607	73.277	1.00	28.98
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20	2294	CA	TYR	В	70	4.00	5 -5.577	74.229	1.00	30.51
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	2298	CE1	TYŔ	В	70	7.639	-3.517	74.670	1.00	29.58
25	2299	CD2	TYR	В	70	5.51	7 -2.133	73.596	1.00	28.94
	2300	CE2	TYR	В	70	6.71	-1.505	73,790	1.00	30.65
	2301	CZ	TYR	В	70	7.758	-2.196	74.326	1.00	30.60
	2302	ОН	TYR	В	70	8.930	-1.537	74.521	1.00	30.30
	2303	С	TYR	В	70	3.65	-5.673	75.723	1.00	34.02
30	2304	0	TYR	В	70	2.86	-4.891	76.259	1.00	33.42
	2305	N	ALA	В	71	4.26	-6.645	76.387	1.00	45.31
	2306	CA	ALA	В	71	4.010	-6.898	77.794	1.00	48.29
	2307	CB	ALA	В	71	4.290	-8.363	78.088	1.00	41.40
	2308	С	ALA	В	71	4.786	-6.020	78.772	1.00	50.20
35	2309	0	ALA	В	71	4.192	2 -5.331	79.601	1.00	50.83
	2310	N	PHE	В	72	6.117	-6.073	78.688	1.00	55.08
	2311	CA	PHE	В	72	7.011	-5.305	79.567	1.00	55.92
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	2313	CG	PHE	В	72	7.970	-5.385	81.935	1.00	49.88
40	2314	CD1	PHE	В	72	7.130	-4.597	82.716	1.00	50.76
	2315	CD2	PHE	В	72	9.322	-5.467	82.274	1.00	49.65
	2316	CE1	PHE	В	72	7.625	-3.912	83.811	1.00	50.29
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5	2365	N	THE		78		11.897	1.452		1.00 67.76
	2366	CA	THE		78		11.929	2.755	86.178	1.00 68.98
•		· CB	THE		78	•	12.236	3.891	85.156	1.00 61.27
	2368	OG1			78		11.110	4.082	84.290	1.00 60.24
	2369	CG2			78		13.449	3.530	84.303	1.00 59.39
- 10	2370	С	THE		78		10.537	2.964	86.778	1.00 69.99
	2371	0	THE		78		10.022		86.869	1.00 69.56
	2372	N	ARG		79		9.941	1.850	87.180	1.00 73.72
	2373	CA	ARG		79		8.603	1.832	87.751	1.00 76.03
	2374	СВ	ARG		79		7.771	0.756	87.034	1.00 80.00
15	2375	CG	ARG		79		6.391	1.197	86.550	1.00 82.26
	2376	CD	ARG		79		6.478		85.368	1.00 84.20
*	2377	NE	ARG	В	79		6.113	1.520	84.097	1.00 86.95
	2378	CZ	ARG	В	79		4.927	0.976	83.837	1.00 89.12
	2379	NH1	ARG	В	79		3.976	0.969	84.761	1.00 89.94
20	2380	NH2	ARG	В	79		4.685	0.452	82.643	1.00 90.19
	2381	С	ARG	В	79		8.703	1.517	89.249	1.00 76.04
	2382	0	ARG	В	79		9.733	1.026	89.709	1.00 75.74
	2383	N	PRO	В	80		7.636	, 1.800	90.024	1.00 79.82
	2384	CD	PRO	В	80		6.375	2.454	89.636	1.00 73.77
25	2385	CA	PRO	В	80		7.634	1.535	91.459	1.00 80.67
,	2386	CB	PRO	В	80		6.179	1.769	91.845	1.00 73.72
	2387	CG	PRO	В	80		5.810	2.890	90.980	1.00 73.71
	2388	С	PRO	В	80		8.115	0.130	91.802	1.00 82.00
	2389	0	PRO	В	80		7.709	-0.859	91.187	1.00 81.64
30	2390	N	ASP	В	81		8.986	0.080	92.804	1.00121.28
	2391	CA	ASP	В	81		9.597	-1.141	93.301	1.00122.10
	239,2	CB	ASP	В	81		10.239	-0.855	94.657	1.00120.79
	2393	CG	ASP	В	81		11.310	-1.850	95.011	1.00122.23
	2394	OD1	ASP	В	81		11.021	-3.061	94.987	1.00122.99
35	2395	OD2	ASP	Þ	81		12.442	-1.420	95.317	1.00123.05
	2396	С	ASP	В	81		8.631	-2.313	93.424	1.00121.97
	2397	0	ASP	В	81		8.986	-3.446	93.105	1.00121.97
	2398	N	GLN		82		7.414	-2.049	93.888	1.00 95.10
	2399	CA	GLN	В	82		6.435	-3.120	94.044	1.00 95.24
40	2400	CB	GLN	В	82		5.402	-2.756	95.109	1.00 96.25
	2401	CG	GLN	В	82		5.943	-2.900	96.534	1.00 97.17
	2402	CD	GLN	В	82		6.653	-4.241	96.776	1.00 97.46
	2403	OE1	GLN	В	82		7.740	-4.490	96.246	1.00 97.11

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	2404	NE	2 GI	N E	82		6.	033	-5.106	97.57	5 1.00	97.19
	2405	C	GL	N E	82		5.	756	-3.522	92.74	7 1.00	94.98
	2406	.0	GL	N E	82		. 5.	577	-4.711	92.48	7 1.00	94.54
	2407	N	GL	U B	83		5.	359	-2.551	91.93	2 1.00	120.68
5	2408	CA	GL	U B	83		4.	778	-2.909	90.64	8 1.00	120.50
	2409	CB	GL	ÜΒ	83		4.	324	-1.667	89.87		93.98
	2410	CG	GL	U B	83	. '	3.	731	-1.984	88.50		93.63
	2411	CD	GL	UВ	83		3.3	334	-0.741	87.73		93.74
	2412	OE	1 GL	UВ	83		3.0	283	-0.849	86.52		93.84
10	2413	OE.	2 GL	U _, B	83		3.2	267	0.346	88.34		94.14
	2414	С	GL	ÜΒ	83		5.9	996	-3.545	89.97		120.39
	2415	0	GL	UВ	83		7.0	087	-3.506	90.54		121.16
	2416	N	VA:	LВ	84	•	. 5.8	339	-4.110	88.785		101.60
	2417	CA	VA:	LВ	84		6.9	951	-4.774			100.63
15	2418	CB	VA	LВ	84		8.1	.97	-3.844			66.48
	2419	CG	L VAI	БΒ	8.4		7.8	12	-2.385	88.071		65.73
	2420	CG2	EAV S	LВ	84		9.3	142	-4.253	88.80		65.12
	2421	C	VAI	ЪВ	84		7.3	66	-6.000	88.902		100.20
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	2425	CB	LYS	ВВ	85		7.8	84	-6.461	92.529		90.57
	2426	CG	LYS	В	85		7.9	88	-7.552	93.577		90.50
	2427	CD	LYS	В	85		. 8.2	44"	-6.935	94:942		92.14
25	2428	CE	LYS	В	85		8.2	66	7.970	96.056		92.89
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	2432	N	PHE	. B	86		5.2	48	-6.979	91.003		02.16
30	2433	CA	PHE	В	86	•	3.89	94	-7.509	90.924	1.001	01.13
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	2435	CG	PHE		86		1.50)9	-6.649	90.743	1.001	14.40
	2436		PHE		86		0.71	L 4	-7.668	91.255	1.001	14.81
	2437		PHE		86		1.00)1	-5.851	89.724	1.001	14.98
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	2603	N	ASN	В	106	-5.453	-24.256	70.689	1.00	42.40
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30	2605	СВ	ASN	В	106	-5.065	-25.049	68.431	1.00	35.23
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35	2610	0	ASN	В	106	-3.160	-22.996	68.383	1.00	41.51
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	2613	CB	VAL	В	107	-2.909	-20.252	71.365	1.00	41.29
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40	2615	CG2	VAL	В	107	-4.224	-19.699	70.861	1.00	39.98
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	2885	0	LEU	В	141	3.006	-16.098	71.857	1.00	36.58
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5	3053	OD2	ASP	в 163	28.313 -16.879	65.985	1.00 84.15
	3054	С	ASP	в 163	30.974 -14.950	63.376	1.00 79.30
	3055	0	ASP	В 163	31.689 -15.757	62.791	1.00 80.39
	3056	N	VAL	B 164	30.986 -13.653	63.086	1.00 67.38
	3057	CA	VAL	B 164	31.882 -13.150	62.046	1.00 68.00
· 10	3058	CB	VAL	B 164	31.707 -11.641	61.800	1.00 68.44
	3059	CG1	VAL	B 164	32.401 -11.250	60.509	1.00 68.71
	3060	CG2	VAL	3 164	30.240 -11.282	61.757	1.00 68.53
	3061	С	VAL I	3 164	33.289 -13.374	62.581	1.00 68.33
	3062	0	VAL	3 164	34.187 -13.823	61.866	1.00 66.84
15	3063	N	TEO 1	3 165	33.449 -13.070	63.863	1.00 80.97
	3064	CA	LEU I	3 165	34.718 -13.216	64.553	1.00 82.49
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	3067	CD1	LEU I	3 165	36.689 -13.655	67.072	1.00 80.94
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	3069	С		3 165	35.213 -14.650	64.419	1.00 82.96
	3070	0	LEU H		36.358 -14.880		1.00 83.85
	3071	N .		3 166	34.349 -15.617		1.00 68.73
05	3072	CA	ASP E		34.746 -17.014	•	1.00 69.37
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	3076		ASP E		34.894 -16.460	·	1.00109.83
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30	3078	0	ASP E		34.388 -18.798	63.055	1.00 68.96
	3079	N			34.861 -16.770		
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	3081	CB	ALA E		36.122 -17.850	60.416	1.00 71.38
35	3082	C	ALA E		33.662 -18.160	60.512	1.00 73.42
33	3083 3084	O N	ALA B		33.684 -18.861	59.503	1.00 73.13
		N Cn	LYS B		32.668 -18.193	61.395	1.00 76.94
	3085	CA	LYS B		31.518 -19.059	61.209	1.00 76.07
	3086	CB	LYS B			62.504	1.00 83.53
40	3087	CG	LYS B			63.741	1.00 84.67
	3088	CD	LYS B		· · · · · · · · · · · · · · · · · · ·	64.821	1.00 86.13
	3089	CE NZ	LYS B		31.271 -20.088	66.201	1.00 85.76
	3090		LYS B			66.753	1.00 86.00
	3091	С	LYS B	Тря	30.638 ÷18.476	60.109	1.00 75.99

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	3094				1,-16.516		1.00	56.70
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5	3096				6 -17.042		1.00	89.46
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	3098				5 -14.129		1.00	89.12
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20	3111	CA	PRO B 171	31.02	0 -9.753	56.819	1.00	78.61
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	3114	С	PRO B 171	30:37	9.330	55.500	1.00	77.50
	3115	O .	PRO B 171.	29.63	68.348	55.447	1.00	78.36
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	3117	CA	GLY B 172	30.049	9.747	53.158	1.00	70.47
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35	3126	С	ASP B 173	26.261	-11.289	55.176	1.00	56.51
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		CDI	ILE B 174	28.680	-7.991		1.00	
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	3138	СВ	THR B 175	22.167 -9.189	53.814	1.00 47.89
5	3139	OG	1 THR B 175	22.080 -10.579	54.141	1.00 47.65
	3140	CG	2 THR B 175	23.292 -8.990	52.830	1.00 47.35
	3141	С	THR B 175	21.157 -8.277	55.894	1.00 47.27
	3142	0	THR B 175	20.968 -8.952	56.907	1.00 48.30
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	3145	CB	GLU B 176	18.082 -6.378	55.237	1.00 38.17
	3146	CG	GLU B 176	18.450 -4.914	55.152	1.00 39.37
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25.	3159	С	GLU B 177	18.532 -11.380		
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	3161	N	LEU B 178	19.857 -11.410		1.00 41.63
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30	3163 3164	CB CG	LEU B 178 LEU B 178	22.134 -11.738		
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	3166		LEU B 178	22.852 -13.711		
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35		N	ILE B 179	20.354 -10.182	60.137	1.00 35.45
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	3266	CE	LYS	В	190	14.436	-16.857	56.654	1.00	67.52
	3267	NZ	LYS	В	190	15.093	-17.892	55.793	1.00	67.17
5	3268	C ·	LYS	В	190	8.902	-15.242	57.073	.1.00	45.92
	3269	0	LYS	В	190	9.076	-14.053	57.308	1.00	45.33
	3270	N .	ASP	В	191	7.821	-15.682	56.453	1.00	41.73
	3271	CA	ASP	В	191	6.824	-14.733	55.996	1.00	41.48
	3272	СВ	ASP	В	191	5.856	-15.402	55.030	1.00	63.45
10	3273	CG	ASP	В	191	6.313	-15.294	53.592	1.00	67.43
	3274	OD1	ASP	В	191	5.676	-15.921	52.717	1.00	70.88
	3275	OD2	ASP	В	191	7.306	-14.577	53.329	1.00	69.09
	3276	С	ASP	В	191	6.042	-14.028	57.070	1.00	40.03
	3277	0	ASP	В	191	5.336	-13.078	56.775	1.00	39.83
15	3278	N	LEU	В	192	6.168	-14.449	58.321	1.00	47.34
	3279	CA	LEU	В	192	5.387	-13.798	59.350	1.00	45.66
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•	3281	CG	LEU	В	192	3.454	-15.563	59.196	1.00	36.65
	3282	CD1	LEU	В	192	2.572	-16.388	60.112	1.00	38.15
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	3284	С	LEU	В	192	6.144	-13.000	60.395	1.00	45.53
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	3291	NE	ARG	В	193	12.214	-14.948	60.547	1.00	44.54
	3292	CZ	ARG	В	193	13.422	-15.261	60.085	1.00	46.24
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40	3303	С	ASP	В	194	5.678	-8.308	60.532	1.00	42.96
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	3309	CG	PRO	В	195		4.930	-6.870	63.642	1.00	30.37
	3310	С	PRO	В	195		3.271	-6.362	60.469	1.00	32.39
5	3311	0	PRO	В	195		3.950	-5.469	59.973	1.00	33.28
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	3313	CA	ASP	В	196		1.407	-5.894	58.967	1.00	33.08
	3314	СВ	ASP	В	196		0.356	-6.723	58.213	1.00	40.99
	3315	CG	ASP	В	196		0.898	-8.031	57.676	1.00	41.96
10	3316	OD1	ASP	В	196		1.002	-9.013	58.450	1.00	42.06
	3317	OD2	ASP	В	196		1.215	-8.063	56.467	1.00	43.06
	3318	С	ASP	В	196	•	0.685	-4.704	59.599	1.00	31.99
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	3323	CG	LEU	В	197		-2.962	-3.590	62.471	1.00	38.39
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	3325	CD2	LEU	В	197		-4.163	-4.514	62.546	1.00	40.85
20	3326	С	LEU	В	197		0.019	-3.762	63.031	1.00	42.42
	3327	0	LEU	В	197		-0.003	-4.757	63.764	1.00	42.95
	3328	N	ILE	В	198		0.445	-2.564	63.438	1.00	34.38
	3329	CA	ILE	В	198		0.887	-2.335	64.807	1.00	3537
	3330	CB	ILE	В	198		2.266	-1.644	•	1.00	26.32
25	3331	CG2					2.471	-0.929	66.202	1.00	23.20
	3332	CG1					3.359	-2.690	64.602		23.88
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	3334	С	ILE				-0.141	-1.456	65.484		36.77
20	3335	0	ILE				-0.430	-0.369	64.981		37.04
30	3336	N	ILE				-0.668	-1.926	66.621	1.00	41.16
	3337	CA	ILE					-1.240			43.74
	3338	СВ			199		-2.941	-2.196			49.23
	3339		ILE				-3.835	-1.671	68.767		45.95
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	3343	0	ILE				-0.899	-1.468	69.652		45.29
	3344	N	ARG				-1.479	0.608	68.953		36.74
40	3345	CA	ARG				-1.182		70.230		37.18
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	3347	CG	ARG				0.216		71.367		45.83
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5	3353					2.597	. / \	1.00 34.80
J	3354	0	ARG I		-2.876	•	71.963	1.00 42.28
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10	3358	OG1		3 201			72.999	1.00 24.68
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25	3373	CA		B 204	-0.020		73.446	1.00 42.47
25	3374	CB		B 204 B 204	-0.020		· · · · ·	
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35	3384	CG		B 205	-0.410			1.00 35.68
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40	3389	N		B 206			70.005	1.00 38.80
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	JJJ2	-	* *****		1.100			

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	3395	CZ	ARG	В	206		4.201	9.012	75.297	1.00	53.40
	3396	NH:	l ARG	В	206		3.557	8.18.9	76.111	1.00	51.40
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	3398	С	ARG	В	206	٠	4.709	5.233	69.988	1.00	40.18
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	3403	CG	LEU	В	207		5.915	2.949	67.024	1.00	37.95
	3404	CD1	LEU	В	207		6.712	3,206	65.771	1.00	37.88
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	3410	CB	SER	В	208		6.946	2.888	73.963	1.00	42.07
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•	3413	0	SER	В	208.		8.811	0.973	73.396	1.00	37.18
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	3415	CA	ASN	В	209		10.670	0.968	.,71.306	1.00	30.52
	3416	CB	ASN	В	209	•	11.650	0.854	72.473	1.00	26.40
25	3417	CG	ASN	В	209		13.036	0.448	72.034	1.00	25.66
	3418	OD1	ASN	В	209		13.800	-0.097	72.808	1.00	27.06
	3419	ND2	ASŅ	В	209		13.372	0.730	70.790	1.00	26.24
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	3421	0	ASN	В	209		10.634	-1.424	71.434	1.00	30.39
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	3424	CB	PHE				6.864	-1.663	70.147	1.00	33.86
	3425	CG	PHE					-2.984		1.00	35.91
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35	3427		PHE				5.266	-3.242	69.020	1.00	36.79
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		3480) и	TYR	B 217		7.827		•		0 33.05
	•	3481	CA	TYR	B 217		6.859	-0.762	57.337	1.0	0 33.52
		3482	CB	TYR'	в 217		7.129				26.97
	5	3483	CG		в 217		8.494		55.375		27.03
		3484	CD:	1 TYR 1	B 217	٠.	9.606	-2.025	55.751		28.49
		3485	CE:	l TYR I	B 217	,	10.823	-1.913	55.083		26.38
		3486	CD2	2 TYR I	3 217		8.657	-0.332	54.325		27.94
		3487	CE2	2 TYR I	3 217	,	9.867	-0.217	53.658		29.81
	10	3488	CZ	TYR I	3 217		10.936	-1.012	54.036	1.00	30.32
		3489	ОН	TYR E	3 217		12.096	-0.935	53.320		35.46
		3490	С	TYR E	3 217		5.435	-1.091	57.710		35.00
		3491	0	TYR E	3 217		4.535				37.26
		3492	N	SER E	3 218		5.202	-1.544	58.935		31.38
	15	3493	CA	SER E	218	•	3.835	-1.880	59.312	. 1.00	34.90
		3494	СВ	SER E	218	•	3.823	-2.590	60.667	1.00	44.37
		3495	OG	SER B	218		4.843	-2.094	61.506	1.00	49.79
		3496	С	SER B	218		2.885	-0.686	59.316	1.00	34.66
		3497	0	SER B	218		3.316	0.460	59.255	1.00	35.96
	20	3498	N	GLU B	219		1.586	-0.980	59.345	1.00	46.39
		3499	CA	GLU B	219		0.540	0.042	59.376	1.00	48.11
		3500	CB	GLU B	219		-0.780	-0.477	58.787	1.00	42.82
		3501	CG	GLU B	219		-0.765	-0.799	57.29 5	1.00	40.25
		3502	CD	GLU B			-0.760		56.421		
	25	3503		GLU B			-0.641	1.561	56.965	1.00	41.05
		3504		GLU B			-0.869	0.295	55.185	1.00	43.48
		3505	С	GLU B			0.305		60.832	1.00	48.55
		3506	0	GLU B					61.651	1.00	49.82
	20	3507	N	LEU B			0.279		61.168		42.65
•	30	3508	CA	LEU B					62.551	1.00	44.53
		3509	CB	LEU B			0.892	3.210	62.912	1.00	34.86
		3510	CG	LEU B			2.283	2.957	63.502	1.00	31.02
		3511		LEU B			2.922	1.740	62.852	1.00	29.61
	25	3512		LEU B			3.133	4.208	63.320	1.00	32.36
	35	3513		LEU B			-1.403	2.250	62.769	1.00	46.39
		3514		LEU B			-2.089	2.722	61.867	1.00	47.21
		3515		TYR B			-1.882	1.929	63.964	1.00	53.95
		3516 \		TYR B			-3.278	2.147	64.310	1.00	55.64
	40	3517		TYR B			-4.115	0.923	63.976	1.00	58.57
	40	3518		TYR B			-5.529		64.477	1.00	60.14
		3519		TYR B			-6.372			1.00	59.26
		3520		TYR B			-7.661			1.00	
		3521	CD2	TYR B	221		-6.012	0.155	65.430	1.00	61.11

	3522	CE2	TYR	В	221		-7.294		0.274	65.930	1.00	62.90
	3523	CZ	TYR	В	221		-8.116		1.283	65.476	1.00	62.23
	3524	ОН	TYR	В	221		-9.384		1.397	66.009	1.00	60.46
	3525	С	TYR	В	221		-3.451		2.471	65.781	1.00	57.07
5	3526	0	TYR	В	221		-3.361		1.586	66.639	1.00	58.08
	3527	N	PHE	В	222		-3.710		3.749	66.050	1.00	56.47
	3528	CA	PHE	В	222		-3.912		4.262	67.402	1.00	57.27
	3529	СВ	PHE	В	222		-3.249		5.630	67.548	1.00	49.96
	3530	CG	PHE	В	222		-1.891		5.695	66.946	1.00	48.78
10	3531	CD1	PHE	В	222		-1.735		5.891	65.589	1.00	47.54
•	3532	CD2	PHE	В	222		-0.760		5.524	67.731	1.00	49.19
	3533	CE1	PHE	В	222		-0.476	•	5.916	65.019	1.00	48.43
	3534	CE2	PHE	В	222		0.504		5.547	67.167	1.00	46.75
	3535	CZ	PHE	. B	222		0.643		5.744	65.810	1.00	47.56
15	3536	С	PHE	В	222	•	-5.393		4.387	67.762	1.00	58.98
	3537	0	PHE	В	222		-6.233		4.773	66.937	1.00	59.22
	3538	N	THR	В	223	•	-5.700		4.074	69.013	1.00	65.91
	3539	CA	THR	В	223	•	-7.064		4.137	69.491	1.00	66.56
	3540	CB	THR	В	223	-	-7.710		2.747	69.429	1.00	68.79
20	3541	OG1			223	-	-9.101		2.874	69.729	1.00	73.73
	3542	CG2	THR	В	223		-7.054		1.784	70.423	1.00	66.05
	3543	С			223		-7.092		4.667	70.921	1.00	67.20
	3544	0			223	-	-6.491		4.077	71.823	1.00	68.64
0.5	3545	N	ASP				-7.793		5.780	71.126	1.00	59.07
25	3546	CA	ASP				-7.875		6.392		.1.00	57.77
•	3547	CB	ASP				-8.771		7.641	72.413		59.96
	3548	CG	ASP		,		-8.166		8.766	71.589		62.19
	3549		ASP				-7.818		8.503	70.421		64.70
30	3550		ASP				-8.031		9.903	72.095		61.88
30	3551	C	ASP				-8.340		5.461	73.569		56.76
	3552	0	ASP				-8.283		5.837	74.737		56.94
	3553	N	THR				8.781		4.249	73.235		40.23
	3554	CA	THR				9.243		3.326	74.275		41.21
35	3555 3556	CB	THR				0.184			73.710		69.35
33	3557		THR THR				9.579		0.943	73.891		71.55
	3558	C	THR				.0.481		2.466	72.240		70.88
	3559	0	THR		·		8.111		2.642	75.033		39.57
	3560	N	LEU.				7.111		2.280	74.443		38.26
40	3561	CA	LEU				8.288		2.478	76.343		49.79
70	3562	CB	LEU				7.297		1.834	77.202		50.45
	3563	CG	LEU				7.552		2.146	78.679		73.50
							7.670		3.606	79:135		75.22
	3564	CDI	LEU	D	220	-	6.975		3.744	80.476	1.00	73.87

	3565	CD2	LEU	В 226	-7.065	4.561	78.114	1.00	73.91
	3566	С	LEU	B 226	-7.346	0.338	77.003	1.00	50.06
	3567	0	LEU	в 226	-8.382	-0.213	76.671	1.00	50.52
	3568	N ·	TRP	в 227	-6.220	-0.317	77.238	1.00	56.52
5	3569	CA	TRP	В 227	-6.109	-1.749	77.031	1.00	55.63
	3570	СB	TRP	B 227	-4.836	-2.282	77.672	1.00	40.08
	3571	CG	TRP	В 227	-4.591	-3.710	77.343	1.00	32.65
	3572	CD2	TRP	В 227	-4.712	-4.336	76.056	1.00	29.73
	3573	CE2	TRP	В 227	-4.357	-5.698	76.220	1.00	29.35
10	3574	CE3	TRP	B 227	-5.086	-3.882	74.778	1.00	30.04
	3575	CD1	TRP	B 227	-4.183	-4.682	78.202	1.00	32.68
	3576	NE1	TRP	B 227	-4.039	-5.877	77.541	1.00	31.63
	3577	CZ2	TRP	B 227	-4.362	-6.616	75.158	1.00	27.35
	3578	CZ3	TRP	B 227	-5.092	-4.802	73.714	1.00	27.85
15	3579	CH2	TRP	B 227	-4.729	-6.154	73.923	1.00	28.92
	3580	С	TRP	B 227	-7.272	-2.637	77.446	1.00	57.42
•	3581	0	TRP	B 227	-7.930	-3.220	76.593	1.00	57.78
	3582	N	PRO	B 228	-7.550	-2.758	78.751	1.00	59.57
	3583	CD	PRO	B 228	-6.949	-2.138	79.942	1.00	82.42
20	3584	CA	PRO	B 228	-8.669	-3.634	79.131	1.00	61.06
	3585	CB	PRO	B 228	-8.747	-3.451	80.649	1.00	84.47
	3586	CG	PRO	B 228	-7.327	-3.129	81.022	1.00	83.95
•	3587	С	PRO	B 228	-9.997	,−3.339	78.417	1.00	60.86
	3588	0	PRO	B 228	-10.852	-4.210	78.278	1.00	59.30
25·	3589	N	ASP	B 229	-10.157	-2.106	77.960	1.00	63.90
	3590	CA	ASP	В 229	-11.363	-1.717	77.257	1.00	65.67
	3591	СВ		В 229	-11.548	-0.203	77.324	1.00	66.08
	3592	CG		B 229	-11.601	0.310	78.741	1.00	67.12
20	3593			В 229	-11.670		78.925		66.03
30	3594	OD2		В 229		-0.527			
	3595	С		В 229		-2.147			
	3596	0		В 229	-12.000	-1.681	74.950		67.93
	3597	N		B 230	-10.289	-3.021	75.523		69.70
25 .	3598	CA		B 230	-10.096	-3.506	•		67.90
35	3599	CB		B 230	-8.606	-3.656	73.841	1.00	
	3600	CG		B 230	-8.283	-3.509	72.382		26.39
	3601			B 230	-8.216	-2.262	71.801	1.00	
	3602			B 230	-8.033		71.589		22.39
40	3603			B 230	-7.901		70.446	1.00	
40	3604			B 230		-4.476	70.236		17.21
	3605	CZ		B 230		-3.215	69.669	1.00	
	3606	С		B 230		-4.859	74.130		70.82
	3607	0	PHE :	В 230	-10.607	-5.682	75.032	1.00	70.34

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	3653	CA	GLU E	3 237		-12.645	-1.703	63.957	1.00	52.29
	3654	СВ	GLU E	3 237		-13.006	-0.707	65.068	1.00	76.60
5	3655	CG	GLU E	3 237		-13.056	0.756	64.605	1.00	78.85
	3656	CD	GLU E	3 237		-14.097	1.005	63.514	1.00	81.46
	3657	OE1	GLU E	3 237		-15.314	1.018	63.822	1.00	81.02
	3658	OE2	GLU E	3 237		-13.690	1.184	62.342	1.00	81.65
	3659	С	GLU E	3 237	,	-11.266	-1.397	63.413	1.00	51.87
10	3660	0	GLU .E	3 237		-11.099	-0.530	62.552	1.00	51,44
	3661	N	ALA E	3 238		-10.287	-2.137	63.929	1.00	63.75
	3662	CA	ALA E	238		-8.892	-1.999	63.532	1.00	62.12
	3663	СВ	ALA E	238		-7.991	-2.450	64.657	1.00	66.94
	3664	С	ALA E	238		-8.636	-2.842	62.297	1.00	60.80
15	3665	0	ALA E	238	•	-8.329	-2.299	61.230	1.00	60.24
	3666	N	ILE E	239	•	-8.758	-4.166	62.453	1.00	40.23
	3667	CA	ILE E	239		-8.555	-5.104	61.348	1.00	39.87
	3668	СВ	ILE E	239		-9.165	-6.492	61.642	1.00	35.32
	3669	CG2	ILE B	239		-8.936	-7.420	60.475	1.00	34.94
20	3670	CG1	ILE B	239		-8.528	-7.092	62.886	1.00	32.97
	3671	CD1	ILE B	23,9	•	-9.005	-8.480	63.222	1.00	31.96
	3672	С	ILE B	239		-9.272	-4.511	60.148	1.00	42.94
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	3674	N	LEU B	240		-10.358	-3.802	60.437	1.00	80.50
25	3675	CA	LEU B	240		-11.155	-3.148	59.417	1.00	83.41
	3676	CB	LEU B	240		-12.435	-2.583	60.025	1.001	108.88
	3677	CG	LEU B	240		-13.154	-1.558	59.145	1.001	10.23
	3678	CD1	LEU B	240		-13.680	-2.234	57.881	1.001	109.99
	3679	CD2	LEU B	240		-14.283	-0.912	59.936	1.001	10.96
30	3680	С	LEU B	240		-10.350	-2.011	58.816	1.00	85.14
	3681	0	LEU B	240		-9.800	-2.134	57.719	1.00	86.33
	3682	N	ALA B	241		-10.285	-0.901	59.544	1.00	88.35
	3683	CA	ALA B	241		-9.556	0.265	59.075	1.00	88.88
	3684	СВ	ALA B	241		-9.279	1.206	60.227	1.00	57.91
35	3685	С	ALA B	241		-8.258	-0.186	58.429	1.00	89.35
	3686	0	ALA B	241		-7.809	0.404	57.450	1.00	89.34
	3687	N	TYR B	242		-7.663	-1.242	58.973	1.00	68.33
	3688	CA	TYR B	242		-6.430	-1.760	58.410	1.00	69.38
	3689	СВ	TYR B	242		-6.063	-3.101	59.040	1.00	61.75
40	3690	CG	TYR B	242		-5.017	-3.847	58.243	1.00	59.73
	3691	CD1	TYR B	242		-3.834	-3.219	57.858	1.00	58.22
	3692	CE1	TYR B	242		-2.886	-3.878	57.083	1.00	57.00
	3693	CD2	TYR B	242		-5.224	-5.164	57.838	1.00	58.12

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       3698
             0
                  TYR B 242
                                 -5.810
                                          -1..486
                                                  56.104
                                                           1.00 70.96
       3699
             N
                  ASN B 243
                                 -7.703
                                                  56.553
                                          -2.621
                                                           1.00 63.54
       3700
             CA
                 ASN B 243
                                 -8.010
                                          -2.862
                                                  55.157
                                                           1.00 65.12
       3701
             CB
                 ASN B 243
                                 -9.069
                                          -3.946
                                                  55.033
                                                           1.00 62.53
       3702
                 ASN B 243
             CG
                                 -8.552
                                          -5.293
                                                  55.444
                                                           1.00 61.37
 10
       3703
             OD1 ASN B 243
                                 -8.995
                                          -5.852
                                                  56.441
                                                           1.00 61.93
       3704
             ND2 ASN B 243
                                 -7.600
                                          -5.826
                                                  54.680
                                                           1.00 61.00
       3705
             С
                 ASN B 243
                                 -8.482
                                          -1.602
                                                  54.451
                                                           1.00 66.20
       3706
                 ASN B 243
                                 -8.280
                                          -1.445
                                                  53.245
                                                          1.00 65.95
       3707
             N
                 ARG B 244
                                 -9.109
                                          -0.701
                                                  55.199
                                                          1.00 64.72
 15
       3708
             CA
                ARG B 244
                                 -9.594
                                           0.540
                                                  54.611
                                                          1.00 67.47
       3709
                 ARG B 244
            CB
                                -10.226
                                          1.424
                                                  55.681
                                                          1.00 94.83
      3710
             CG
                 ARG B 244
                                -11.040
                                          2.574
                                                  55.119
                                                          1.00 96.30
      3711
             CD
                 ARG B 244
                                -12.422
                                          2.113
                                                  54.689
                                                          1.00 98.16
      3712
             NE
                 ARG B 244
                                -13.377
                                          2.045
                                                  55.803
                                                          1.00 99.54
 20
      3713
             CZ
                 ARG B 244
                                -13.363
                                          1.139
                                                  56.781
                                                          1.00 99.23
      3714
            NH1 ARG B 244
                                -12.436
                                          0.191
                                                  56.810
                                                          1.00 99.50
      3715
            NH2 ARG B 244
                                -14.286
                                          1.181
                                                  57.734
                                                          1.00 98.66
      3716
            С
                 ARG B 244
                                -8.435
                                          1.290
                                                  53.961
                                                          1.00 69.17
      3717
            0
                 ARG B 244
                               -8.625
                                          2.043
                                                 53.006
                                                          1.00 69.16
25
      3718
            Ν
                 ARG B 245
                                -7.231
                                          1.078
                                                 54.483
                                                          1.00 90.19
      3719
                ARG B 245
            CA
                                -6.046
                                          1.746
                                                 53.960
                                                          1.00 92.43
      3720
            CB
                ARG B 245
                                -4.814
                                          1.401
                                                 54.805
                                                          1.00 79.40
      3721
            CG
                ARG B 245
                                -5.013
                                          1.508
                                                 56.315
                                                          1.00 78.40
      3722
            CD
                ARG B 245
                                -5.394
                                          2.918
                                                 56.755
                                                         1.00 78.14
30
      3723
            NE
                ARG B 245
                                -5.540
                                          3.030
                                                 58.208
                                                         1.00 77.20
      3724
            CZ
                ARG B 245
                                -4.539
                                          2.903
                                                 59.078
                                                         1.00 76.66
     3725
            NH1 ARG B 245
                                -3.306
                                          2.658
                                                 58.650
                                                         1.00 76.13
     3726
            NH2 ARG B 245
                                -4.771
                                          3.019
                                                 60.379
                                                         1.00 75.87
     3727
            С
                ARG B 245
                                -5.791
                                          1.326
                                                 52.522
                                                         1.00 94.57
35
     3728
            0
                ARG B 245
                                -5.595
                                                 52.235
                                          0.147
                                                         1.00 94.29
     3729
           N
                HIS B 246
                                -5.813
                                          2.293
                                                 51.617
                                                         1.00142.27
     3730
           CA
                HIS B 246
                                -5.547
                                          2.018
                                                 50.213
                                                         1.00144.64
     3731
           CB
                HIS B 246
                                -6.640
                                         2.603
                                                 49.304
                                                         1.00124.13
     3732
           CG
                HIS B 246
                                -8.010
                                         2.052
                                                 49.544
                                                         1.00125.01
40
           CD2 HIS B 246
     3733
                                -9.171
                                         2.669
                                                 49.869
                                                         1.00125.08
     3734
           ND1 HIS B 246
                                -8.313
                                         0.715
                                                 49.402
                                                         1.00125.24
     3735
           CE1 HIS B 246
                                -9.602
                                         0.532
                                                 49.627
                                                         1.00125.20
     3736
           NE2 HIS B 246
                              -10.145
                                         1.702
                                                 49.912
                                                         1.00125.75
```

	3737	. С	HIS B	246	-4	. 250	2.744	49.899	1.00	0145.61
	3738	0	HIS B	246	-3	.154	2.346	50.307		146.34
	3739	N	ARG B	247	-4	. 434	3.837	49.171		74.46
	3740	CA	ARG B	247	-3	.401	4.755	48.712	1.00	74.85
5	3741	СВ	ARG B	247	-2	260	4.001	48.003	1.00	74.20
	3742	CG	ARG B	247	-2	692	2.816	47.140	1.00	72.35
	3743	CD	ARG B	247	-1.	503	1.878	46.868	1.00	71.58
	3744	NE	ARG B 2	247	-1.	904	0.644	46.187	1.00	70.02
	3745	CZ	ARG B 2	247	-2.	762	-0.249	46.681	1.00	69.37
- 10	3746	NHI	L ARG B 2	247	-3.	322	-0.059	47.871	1.00	69.43
	3747	NH2	ARG B 2	247	· -3.	075	-1.331	45.976	1.00	67.98
	3748	С	ARG B 2	247	-4.	187	5.644	47.750	1.00	75.12
	3749	0	ARG B 2	247	-3.	634	6.502	47.058	1.00	74.84
	3750	N	ARG B 2	248	-5.	505	5.424	47.755	1.00	75.10
15	3751	CA	ARG B 2	248	-6.	450	6.146	46.914	1.00	74.94
	3752	CB	ARG B 2	248	-6.	517	7.627	47.328	1.00	73.91
	3753	CG	ARG B 2		-7.	534	8.433	46.515	1.00	72.01
	3754	CD	ARG B 2		-7.	514	9.937	46.808	1.00	69.76
20	3755	NE	ARG B 2		-8.		10.702	45.719	1.00	67.75
20	3756	CZ	ARG B 2				10.538		1.00	67.22
	3757		ARG B 2				9.633		1.00	66.89
	3758		ARG B 2			827	11.265			65.91
	3759	С	ARG B 2			053	•	45.437		
25	3760	0	ARG B 2				6.997	•		75.09
25	3761	N	PHE B 2				4.758			75.96
	3762	CA	PHE B 2				4.469			76.80
	3763	CB	PHE B 2			998				76.98
	3764	CG	PHE B 2				2.031			
30	3765		PHE B 2				1.945			
50	3766		PHE B 2		-5.		1.177	45.203		
	3767		PHE B 2			310				77.84
	3768 3769	CEZ	PHE B 2		-5.0		0.250	46.008		77.54
	3770	C	PHE B 2		-7. (0.173	45.968		77.55
35	3771	0	PHE B 2		-6.		4.658	42.614		77.29
33	3772	OT	PHE B 24		-7.(3.708	41.838		77.59
	3773		IPP C	1	-7.3		5.763	42.625		77.59
	3774		IPP C	1	3.7		-1.490	77.726		33.83
	3775		IPP C	1	2.8		-0.835	78.560		33.83
40	3776		IPP C	1		16	-2.798	78.081		33.83
.0	3777		IPP C	1		197 _. 175	-0.941 0.215	76.373		33.83
	3778		IPP C	1			3.852	76.421		33.83
	3779		IPP C	1			2.417	77.104		33.83
	3.13	110	-11 0	-	4.0	21	7.411	77.787	1.00	33.83

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3780	O16 IPP C	1	6.225	2.006	78.323	1.00 33.83
3781	O17 IPP C	1	4.317	1.406	76.629	1.00 33.83
3782	O18 IPP C	1 '	, 3.695 ,	2.471	78.827	1.00 33.83

	3780	016	IPP	Ċ	1		6.225	2.006	78.323	1.00	33.83
	3781	017	IPP	C.	1		4.317	1.406	76.629	1.00	33.83
	3782	018	IPP	С	1		, 3.695	2.471	78.827	1.00	33.83
	3783	P19	IPP	Ċ	1		5.684	5.144	77.406	1.00	33.83
5	3784	020	IPP	c .	1		7.110	4.945	76.880	1.00	33.83
	3785	021	IPP'	С	1		4.994	6.358	76.768	1.00	33.83
	3786	022	IPP	С	1		5.646	5.185	78.935	1.00	33.83
	3787	C01	IPP	С	2		2.307	-3.138	81.526	1.00	33.83
•	3788	C02	IPP	c	2		3.668	-3.126	81.578	1.00	33.83
10	3789	C05	IPP	С	2		1.513	-4.452	81.609	1.00	33.83
	3790	C09	IPP	С	2		1.487	-1.841	81.385	1.00	33.83
	3791	C12	IPP	С	2	ė	1.887	-0.699	82.354	1.00	33.83
	3792	014	IPP	С	2		-0.767	2.198	82.197	1.00	33.83
	3793	P15	IPP	С	2		0.246	1.188	81.498	1.00	33.83
15	3794	016	IPP	С	2		-0.425	0.460	80.333	1.00	33.83
	3795	017	IPP	С	2		0.736	0.134	82.638	1.00	33.83
	3796	018	IPP	С	2	•	1.498	2.051	81.154	1.00	33.83
	3797	P19	IPP	C.	2		-1.027	3.757	81.972	1.00	33.83
	3798	020	IPP	С	2		-0.542	4.097	80.558	1.00	33.83
20	3799	021	IPP	С	2		-2.512	4.040	82.143	1.00	33.83
	3800	022	IPP	С	2		-0.165	4.429	83.060	1.00	33.83
	3801	OH2	WAT	W	, 1		12.965	-11.206	62.097	1.00	33.83
	3802	OH2	WAT	M	2		11.962	-27.690	81.314	1.00	33.83
	3803	OH2	WAT	W	3.	: · · .	2.139	4.914	· 78 · 332 ·	1.00	33.83
25	3804	OH2	WAT	W	4		14.094	-9.399	58.598	1.00	33.83
	3805	OH2	TAW	W	5	• • •	12.062	14.669	72.584	1.00	33.83
	END							٠			

Table IIA. Interatomic distances in the native UPPS structure

	rable	IIA. Interat	omic dista	nces in	the native UP	PS structu	ıre
	FROM TO	DIS	TANCE,		27CE	71N	3.956
		A	ngstrom	45	27C	270	1.230
5	27N	27CA	1.470		27C	28N	1.328
	27N	27CB	2.442		27C	27CA	1.515
	27N	27C	2.480		27C	28CA	2.451
	27N	27CG	2.947		27C	27N	2.480
	27N	28N	3.122	50	27C	27CB	2.501
10	27N	700	3.142	į	27C	28C	3.406
	27N	270	3.285		27C	28CB	3.563
	27CA	27N	1.470		27C	280	3.753
	27CA	27C	1.515		27C	27CG	3.873
	27CA	27CB	1.531	55	270	27C	1.230
15	27CA	270	2.394		270	28N	2.255
	27CA	28N	2.404	•	270	27CA	2.394
	27CA	27CG	2.545		270	27CB	2.749
	27CA	28CA	3.793		270	28CA	2.816
	27CA	700	3.988	60	270	27N	3.285
20	27CB	27CG	1.526		270	72N	3.332
	27CB	27CA	1.531		270	72CA	3.576
	27CB	27N	2.442		270	28C	3.674
	. 27CB	27C	2.501	,*	270	72CB	3.836
	27CB	270	2.749	65	. 28N	27C	1.328
25	27CB	27SD	2.828		28N	28CA	1.456
	27CB	27CE	3.129		28N	270	2.255
	27CB	28N	3.678		28N	28CB	2.396
	27CB	700	3.850		28N	27CA	2.404
	27CG	27CB	1.526	70	28N	28C	2.490
30	27CG	27SD	1.817		28N	280	2.808
	27CG	27CA	2.545	÷	28N	27N	3.122
	27CG	27CE	2.831		28N	28CG	3.615
	27CG	27N	2.947		28N	29N	3.640
	27CG	27C	3.873	75	28N	27CB	3.678
35	27SD	27CG	1.817	•	28CA'	28N	1.456
	27SD	27CE	1.863		28CA	28CB	1.524
	27SD	27CB	2.828		28CA	28C	1.546
	27CE	27SD	1.863		28CA	280	2.410
	27CE	27CG	2.831	80	28CA	27C	2.451
40	27CE	27CB	3.129		28CA	29N	2.466
	27CE	700	3.804		28CA	28CG	2.518
	27CE	71CA	3.877		28CA	270	2.816
	27CE	70C	3.929		28CA	280D1	3.045
	•			400			

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	28CA	280D2	3.384		_ 28C	27C	3.406
	28CA	27CA	3.793	45	28C	28CG	3.411
	28CA	29CA	3.824	4	28C	280D1	3.456
	28CA	72CD1	3.860		28C	29C	3.518
5	28CB	28CG	1.490		28C	270	3.674
	28CB	28CA '	1.524		' 28C	30N	3.732
	28CB	280D2	2.338	50	280	28C	1.228
	28CB	280D1	2.356		280	29N	2.239
	28CB	28N	2.396		280	28CA	2.410
10	28CB	28C	2.500		280	29CA	2.711
	28CB	280	3.169		280	28N °	2.808
	28CB	29N	3.287	55	280	28CB	3.169
	28CB	27C	3.563	'	280	29C	3.724
	28CG	280D1	1.240		280	2,7C	3.753
15	28CG	280D2	1.244		29N	28C	1.331
	28CG	28CB	1.490		29N	29CA	1.458
	28CG	28CA	2.518	60	29N	280	2.239
	28CG	72CD1	3.356	• .	29N	28CA	2.466
	28CG	28C	3.411		29N	29C	2.585
20	28CG	72CE1	3.411		· 29N	30N	2.897
	28CG	28N,	3.615		29N	28CB	3.287
	28CG	29N	3.697	65	29N	280D1	3.296
	280D1	28CG	1.240		29N	28N	3.640
	280D1	280D2	2.190	" 1	29N	290	3.691
25	280D1	28CB	2.356	•	29N	28CG	3.697
	280D1	72CE1	2.694		29CA	29N	1.458
	280D1	28CA	3.045	70	29CA	29C	1.520
	280D1'	72CD1	3.057		29CA	290	2.380
	280D1	29N	3.296		29CA	28C .	2.410
30	280D1	28C	3.456		. 29CA	30N	2.454
	280D1	72C2	3.710		29CA	280	2.711
	280D2	28CG	1.244	75	29CA	30CA	3.802
	280D2	280D1	2.190		29CA	28CA	3.824
	280D2	28CB	2.338		29C	290	1.234
35	280D2	28CA	3.384		29C	30N	1.333
	280D2	72CD1	3.624		29C	29CA	1.520
	280D2	72CE1	3.724	80	29C	30CA	2.408
•	28C	280	1.228		29C	29N	2.585
	28C	29N	1.331		29C	30C	2.963
40	28C	28CA	1.546		29C	31N	3.163
	28C	29CA	2.410	* **	29C	28C	3.518
	28C	28N	2.490	85	29C	. 30CB	3.696
	28C	28CB	2.500		29C	280	3.724

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	29C	30ND2	3.761		30CB	300	3.224
	29C	300	3.854	45	30CB	45CD2	3.655
	290	29C	1.234		30CB.	29C	3.696
	290	30N	2.247		30CG	300D1	1.229
5	290	29CA	2.380		30CG	30ND2	1.311
	290	30CA	2.717		30CG	30CB	1.496
	290	30C	2.845	50	30CG	30CA -	2.502
	290	. 31N	3.224		30CG	30N	2.971
	290	300	3.391		30CG	30C	3.825
10	290	, 32N	3.461		30CG	45CD2	3.961
	290	29N	3.691		300D1	30CG	1.229
	290	32C ·	3.973	55 ,	300D1	30ND2	2.230
	30N	29C	1.333		300D1	30CB	2.380
	30N	30CA	1.452		300D1	45CD2	3.392
15	30N	290	2.247		300D1	30CA	3.656
	30N	30CB	2.444		300D1	45CA	3.772
	30N	29CA	2.454	60	30ND2	30CG	1.311
	30N	30C	2.470		30ND2	300D1	2.230
	30N	30ND2	2.764		30ND2	30CB	2.380
20	30N	31N .	2.805		30ND2	30CA	2.652
	30N	29N	2.897		30ND2	30N	2.764
	30N	30CG	2.971	65	30ND2	29C	3.761
	, 30N	. 300.	. 3.526	1.7	. ; a 30C _c -	300	1.229
•	30N	28C	3.732		30C	31N	1.336
25	. 30CA	30N	1.452		30C.	30CA	1.527
	30CA	30CB	1.518		30C	31CA	2.435
	30CA	30C	1.527	70	30C	30N	2.470
	30CA	300	2.391		30C	30CB	2.480
	30CA	29C	2.408		30C	290	2.845
30	30CA	31N	2.442		30C	29C	2.963
	30CA	30CG	2.502		30C	31C	3.116
	30CA	30ND2	2.652	75	30C	32N	3.583
	30CA	290	2.717	•	30C	30CG	3.825
~ =	30CA	300D1	3.656		30C	310	3.839
35	30CA	29CA	3.802		300	30C	1.229
	30CA	31CA	3.812		300	31N	2.256
	30CB	30CG	1.496	80	300	30CA	2.391
	30CB	30CA	1.518		300	31CA	2.775
40	30CB	300D1	2.380		300	31C	3.111
40	30CB	30ND2	2.380		300	30CB	3.224
	30CB	30N	2.444		300	290	3.391
	30CB	30C	2.480	85	300	310	3.441
	30CB	31N	3.172		300	30N	3.526

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	300	32N	3.804		32N	31CA	2.431		
	300	29C	3.854	45	32N	32C	2.438		
	31N	30C	1.336		32N	32CB	2.466		
•	31N	31CA	1.454		32N	31N	2.938		
5	31N	300	2.256	•	32N	32CG	3.309		
	31N	30CA	2.442		32N	290	3.461		
	31N	31C	2.491	50	32N	320	3.504		
	31N	30N	2.805		32N	30C	3.583		
	31N	32N	2.938		32N	300	3.804		
10	31N	29C	3.163		32CA	32N	1.457		
	31N	30CB	3.172		32CA	32C	1.531		
	31N	290	3.224	55	32CA	32CB	1.534		
	31N	310	3.471		32CA	320	2.397		
	31CA	31N	1.454		32CA	31C	2.434		
15	31CA	31C	1.515		32CA	. 32CG	2.585		
	31CA	310	2.378		32CA	310	2.775		
	31CA	32N	2.431	60	32CA	31CA	3.803		
	31CA	30C	2.435		32CA	32CD	3.927		
	31CA	300	2.775		32CB	32CG	1.531		
20	31CA	32CA	3.803		32CB	32CA	1.534		
	31CA	30CA	3.812		32CB	32N	2.466		
	31C	310	1.230	65	32CB	32C	2.495		
•	31C	32N	1.331		32CB	32CD	2.539		
	31C	31CA	1.515	.,	32CB	32NE	3.067		
25	31C	32CA	2.434		32CB	320	3.244		
	31C	31N	2.491		32CB	31C	3.727		
	31C	32C	2.939	70	32CG	32CB	1.531		
	31C	300	3.111		32CG	32CD	1.535		
20	31C	30C	3.116		32CG	32NE	2.519		
30	31C	32CB	3.727		32CG	32CA	2.585		
	31C	320	3.847		32CG	32N	3.309		
	310	31C	1.230	75	32CG	32CZ	3.766		
	310	32N	2.253		32CG	32C	3.838		
25	310	31CA	2.378		32CD	32NE	1.467		
35	310	32CA	2.775		32CD	32CG	1.535		
	310	32C	2.870	00	32CD	32CZ	2.476		
	310	320	3.433	80	32CD	32CB	2.539		
	310	300	3.441		32CD	32NH1	2.829		
40	310	31N ,	3.471	•	32CD	32NH2	3.686		
40	310	30C	3.839		32CD	32CA	3.927		
	32N	31C	1.331	0.5	32NE	32CZ	1.336		
	32N	32CA	1.457	85	32NE	32CD	1.467		
	32N	310	2.253		32NE	32NH1	2.311		

W	0 03/048733					PCT	T/US02/38715
	32NE	32NH2	2.314		45CA	45ND1	3.589
	32NE	32CG	2.519	45	45CA	300D1	3.772
	32NE	32CB	3.067		45CB	45CG	1.497
	32CZ	32NH2	1.329		45CB	45CA	1.532
5	32CZ	32NH1	1.329	•	45CB	45N	2.449
	32CZ	32NE	1.336		45CB	45ND1	2.527
	32CZ	32CD	2.476	50	45CB	45C	2.535
	32CZ	32CG	3.766		45CB	45CD2	2.596
	32NH1	32CZ	1.329		45CB	450	3.264
10	32NH1	32NH2	2.292		45CB	45CE1	3.631
	32NH1	32NE	2.311		45CB	45NE2	3.673
	32NH1	32CD	2.829	55	45CG	45CD2	1.356
	32NH2	32CZ	1.329		45CG	45ND1	1.379
	32NH2	32NH1	2.292		45CG	45CB	1.497
15	32NH2	32NE	2.314		45CG	45NE2	2.200
	32NH2	32CD	3.686		45CG	45CE1	2.206
	32C	320	1.226	60	45CG	45CA	2.520
	32C	32CA	1.531		45CG	45N	2.975
	· 32C	32N	2.438		45CG	45C	3.865
20	32C	32CB	2.495		45CD2	45CG.	1.356
	32C	310	2.870		45CD2	45NE2	1.376
	32C	31C	2.939	65	45CD2	45ND1	2.185
•	32C	32CG	3.838		45CD2	45CE1	2.195
	32C	290	3.973		45CD2	45CB	2.596
· 25	320	32C	1.226		45CD2	45CA	3.208
	320	32CA	2.397		45CD2	300D1	3.392
	320	32CB	3.244	70	45CD2	30CB	3.655
	320	310	3.433		45CD2	45N	3.660
0.	320	32N	3.504		45CD2	30CG	3.961
30	320	31C	3.847		45ND1	45CE1	1.322
	45N	45CA	1.457		45ND1	45CG	1.379
	45N	45C		75°	45ND1	45NE2	2.145
	45N	45CB	2.449		45ND1	45CD2	2.185
	45N	45CG	2.975		45ND1	45CB	2.527
-35	45N	450	3.510		45ND1	45CA	3.589
	45N	45ND1	3.612		45ND1	45N	3.612
	45N	45CD2	3.660	80	45CE1	45NE2	1.322
	45CA	45N	1.457		45CE1	45ND1	1.322
	45CA	45C	1.515		45CE1	45CD2	2.195
40	45CA	45CB	1.532		45CE1	45CG	2.206
	45CA	450	2.382	o =	45CE1	45CB	3.631
	45CA	45CG	2.520	85	45NE2	45CE1	1.322
	45CA	45CD2	3.208		45NE2	45CD2	1.376

W	O 03/048733					PC	T/US02/38715
	45NE2	45ND1	2.145		480	49CA	2.787
	45NE2	45CG	2.200	45	480	52N	2.961
	45NE2	45CB	3.673		480	49C	2,992
	45C	450	1.219		480	48N	3.474
5	45C	45CA	1.515		480	490	3.497
	45C	45N	2.445		480	52CB	3.661
	45C	45CB	2.535	50	480	52CA	3.871
	45C	48N	3.564		49N	48C	1.339
	45C	45CG	3.865		49N	49CA	1.467
10	450	45C	1.219	•	49N	480	2.266
	450	45CA	2.382		49N	48CA	2.435
	450	49N	2.958	55	, 49N	49C	2.446
	450	48N	3.126	•	49N	49CB	2.492
	450	45CB	3.264		49N	48N	2.721
15	450	45N	3.510		. 49N	450	2.958
	450	48CA	3.519	***	4 9 N	49CG	3.422
	450	48C	3.661	60	4 9N	490	3.509
	450	49CB	3.852		49CA	49N	1.467
	450	49CA	3.942		49CA	49C	1.533
20	48N	48CA	1.449		49CA	49CB	1.539
	48N	48C	2.409		49CA	490	2.409
	48N	4 9 N	2.721	65	49CA	48C	2.446
	48N	450	3.126		49CA	49CG	2.603
	48N "	480	3.474		49CA	480	2.787
25	48N	45C	3.564		49CA	48CA	3.814
	48CA	48N	1.449		49CA	450	3.942
	48CA	48C	1.513	70	49CB	49CG	1.527
	48CA	480	2.379		49CB	49CA	1.539
20	48CA	49N	2.435		49CB	. 49N	2.492
30	48CA	450	3.519		4 9CB	49C	2.502
	48CA	49CA	3.814	<i>a.</i> 5	4 9CB	49SD .	2.839
	48C	480	1.235	75	4 9CB	490	3.272
	48C	49N	1.339		49CB	49CE	3.332
35	48C	48CA	1.513		49CB	48C	3.755
55	48C 48C	48N	2.409		49CB	450	3.852
	48C	49CA	2.446	90	4 9CG	49CB	1.527
	48C	49C	3.014	80	4 9CG	49SD	1.852
	48C	450	3.661		49CG	49CA	2.603
40	48C	49CB	3.755		49CG	49CE	2.722
-r ∪	48C 48O	490 48C	3.882		4 9 C G	49N	3.422
	480	48C 49N	1.235	85	49CG	49C	3.813
	480	49N 48CA	2.266	υJ	49SD	49CE	1.728
	400	4 OCA	2.379		49SD	49CG	1.852

W	O 03/048733					PC	CT/US02/38715
	49SD	49CB	2.839	٠,	52CB	52CD1	2.516
	49CE	49SD	1.728	45	52CB	52CD2	2.530
	49CE	49CG	2.722		52CB.	520	3.325
	49CE	49CB	3.332		52CB	490	3.590
5	49C	490	1.232	•	52CB	480	. 3.661
	49C	49CA	1.533		52ÇG	52CD1	1.528
	49C	49N	2.446	50	52CG	52CD2	1.531
	49C	. 49CB	2.502		52CG	52CB	1.545
	49C	480	2.992		52CG	52CA	2.602
10	49C	. 48C	3.014		52CG	52Ç	3.070
	49C	52N	3.736		52CG	520	3.399
	49C	49CG	3.813	55 ,	. 52CG	52N	3.887
	490	49C	1.232		52CD1	52CG	1.528
	490	49CA	2.409		52CD1	52CD2	2.502
15	490	49CB	3.272		52CD1	52CB	2.516
	490 ,	52N	3.272		52CD1	52CA	3.017
	490	480	3.497	60	52CD1	. 520	3.563
	490	49N	3.509		52CD1	52C	3.612
	490	52CB	3.590		52CD2	52CG	1.531
20	490	52CA	3.712	•	52CD2	52CD1	2.502
	. 490	5.2C	3.774		52CD2	52CB	2.530
	490	48C	3:882	65	52CD2	52CA	3.936
	. 52N	52CA	. 1.462		.:	520 .	1.227
	52N	52C	2.431		52C	52CA	1.519
25	52N	52CB	2.493		52C	52N	2.431
	52N .	480	2.961		, 52C	52CB	2.510
	52N	490	3.272	70	52C	52CG	3.070
	52N	520	3.446		52C	52CD1	3.612
	52N	49C	3.736		52C	490	3.774
30	52N	52CG	3.887		520	52C	1.227
	52CA	52N	1.462		520	52CA	2.385
	52CA	52C	1.519	75	520	52CB	3.325
	52CA	52CB	1.544	•	520	52CG	3.399
	52CA	520	2.385		520	52N	3.446
35	, 52CA	52CG	2.602		520	52CD1	3.563
	52CA	52CD1	3.017		70N	70CA	1.453
	52CA	490	3.712	80	70N	70CB	2.386
	52CA	480	3.871		70N	70C	2.439

70N

70N

70N

70CA

70CA

700

71N

7,0CG

70N

70CB

2.904

3.442

3.785

1.453

1.517

3.936

1.544

1.545

2.493

2.510

52CA

52CB

52CB

52CB

52CB

40

52CD2

52CA

52CG

52N

52C

W	/O 03/048733					PC	T/US02/38715
	70CA	70C	1.519		70CE1	70CD2	2.772
	70CA	700	2.393	45	70CE1	70CB	3.808
	70CA	71N	2.421		70CD2	70CE2	1.380
	70CA	70CG	2.582		70CD2	70CG	1.392
5	70CA	70CD1	3.068	1	70CD2	70CD1	2.387
	70CA	70CD2	3.793		70CD2	70CZ	2.394
	70CA	71CA	3.804	50	70CD2	70CB	2.510
	70CB	70CG	1.502		70CD2	70CE1	2.772
	70CB	70CA	1.517		70CD2	700н	3.639
10	70CB	70N	2.386		70CD2	70CA	3.793
	70CB	70C	2.487		70CE2	70CD2	1.380
	70CB	70CD2	2.510	55	70CE2	70CZ	1.385
	70CB	70CD1	2.521		70CE2	700н	2.380
	70CB	700	2.952		70CE2	70CE1	2.396
15	70CB	71N	3.466		70CE2	70CG	2.414
	70CB	70CE2	3.780		. 70CE2	70CD1	2.760
	70CB	70CE1	3.808	60	70CE2	70CB	3.780
	70CG	70CD1	1.391		70CZ	700H	1.367 .
	70CG	70CD2	1.392		70CZ	70CE1	1.376
20	70CG	70CB	1.502		70CZ	70CE2	1.385
	70CG	70CE2	2.414		70CZ	70CD1	2.394
	70CG	70CE1	2.432	65	70CZ	70CD2	2.394
	70CG	70CA	2.582		70CZ	70CG	2.791
	70CG	70CZ	2.791		700Н	70CZ	1.367
25	70CG	70C	3.132		700н	70CE1	2.371
	70CG	700	3.664		700н	70CE2	2.380
	70CG	71N	3.713	70	700H	70CD2	3.639
	70CG	70N	3.785		700н	70CD1	3.644
20	70CD1	70CG	1.391		70C	700	1.238
30	70CD1	70CE1	1.400		70C	71N	1.321
	70CD1	70CD2	2.387		70C	70CA	1.519
	70CD1	70CZ	2.394	75 .	70C	71CA	2.436
	70CD1	70CB	2.521		70C	70N	2.439
25	70CD1	70CE2	2.760		70C	70CB	2.487
35	70CD1	70CA	3.068		70C	71C	3.127
	. 70CD1	70C	3.613	00	70C	70CG	3.132
	70CD1	700H	3.644	80	70C	72N	3.541
	70CD1	71N	3.740		70C	70CD1	3.613
40	70CE1 70CE1	70CZ	1.376		70C	71CB	3.684
40	70CE1	70CD1	1.400		70C	710	3.882
	70CE1	70ОН 70СЕ2	2.371 2.396	85	70C	27CE	3.929
	70CE1	70CE2 70CG	2.432	O)	700	70C	1.238
	, 0022	, 000	2,434		700	71N	2.251

W	0 03/048733					PC	Г/US02/3871
	700	70CA	2.393		71C	72CA	2.475
	700	71CA	2.782	45	71C	71CB	2.505
	700	70N	2.904		71C	71N	2.507
	700	70CB	2.952		71C	70C	3.127
5	700	72N	3.044	•	71C	700	. 3.133
	700	71C	3.133		71C	72CB	3.251
	700	27N	3.142	50	710	71C	1.236
	700	. 70CG	3.664	,	710	72N	2.274
	700	27CE	3.804		710	71CA	2.415
10	700	. 27CB	3.850		710	72CA	2.843
	700	27CA	3.988		710	71CB	2.849
	71N	70C	1.321	55 .	710	71N	3.137
	71N	71CA	1.462		710	72CB	3.448
,	71N	700	2.251		710	70C	3.882
15	71N ·	70CA	2.421		72N	· 71C	1.342
	71N ,	71CB	2.434		72N	72CA	1.470
	71N	71C	2.507	60	'72N	710	2.274
	71N	710	3.137		. 72N	72CB	2.456
	71N	72N	3.354		72N	71CA	2.459
20	71N	70N.	3.442		72N	700	3.044
	71N	70 <u>C</u> B	3.466		72N	270	3.332
	71N	70CG	3.713	65	72N	71N	3.354
	. 71N	70CD1.	3.740		.;	70C	3.541
	71N	27CE	3.956		72N	71CB	3.608
25	71CA	71N	1.462		72N	72CG	3.820
	71CA	71CB	1.517		72CA	72N	1.470
	71CA	71C	1.549	70	72CA	72CB	1.536
,	71CA	710	2.415		. 72CA	71C	2.475
	71CA	70C	2.436		72CA	72CG	2.554
30	71CA	72N	2.459		72CA	710	2.843
	71CA	700	2.782		72CA	72CD2	3.379
	71CA	70CA	3.804	75	72CA	72CD1	3.398
	71CA	72CA	3.860		72CA	270	3.576
	71CA	27CE	. 3.877		72CA	71CA	3.860
35	71CB	71CA	1.517		72CB	72CG	1.507
	71CB	71N	2.434		72CB	72CA	1.536
	71CB	71C	2.505	80	72CB	72N	2.456
	71CB	710	2.849		72CB	72CD2	2.513
	71CB	72N	3.608		72CB	72CD1	2.518
40	71CB	70C	3.684		72CB	71C	3.251
	71C	. 710	1.236		72CB	710	3.448
	71C	72N	1.342	85	72CB	72CE2	3.802

72CB

72CE1

3.806

1.549

71C

71CA

•	WO 03/048733					PC	CT/US02/3871
	72CB	270	3.836		72CZ	72CE1	1.384
	72CG	72CD2	1.387	45	72CZ	72CD2	2.406
	72CG	72CD1	1.388		72CZ	72CD1	2.410
	72CG	72CB	1.507		72CZ	72CG	2.799
5	72CG	72CE2	2.420		72CZ	280D1	3.710
	72CG	72CE1	2.421		72C	72CA	1.526
	72CG	72CA	2.554	50	72C	72N	2.477
	72CG	72CZ	2.799		72C	72CB	2.499
	72CG	72N	3.820		72C	710	2.651
10	72CD1	72CG	1.388		72C	71C	2.881
	72CD1	72CE1	1.398		72C	72CG	3.042
	72CD1	72CD2	2.388	55	72C	72CD2	3.243
	72CD1	72CZ	2.410		720	72CA	2.410
	72CD1	72CB	2.518		720	72CB	3.415
15	72CD1	72CE2	2.769		720	72N	3.450
	72CD1	280D1	3.057		720	72CG	3.541
	72CD1	28CG	3.356	60	['] 720	72CD2	3.581
	72CD1	72CA	3.398		720	710	3.734
	72CD1	28OD2	3.624		720	71C	3.950
20	72CD1	28CA	3.860		90CD1	45CB	3.755
	72CD2	72CG	1.387		90CD2	49CE	3.288
	72CD2	72CE2	1.396	65	900	49SD	3.899
	72CD2	72CD1	2.388		94N	49SD	3.988
	72CD2	72CZ	2.406		94CA	49SD	3.982
25	72CD2	72CB	2.513		·143CE2	52CD2	3.572
•	72CD2	72CE1	2.767		143CZ	52CD2	3.734
	72CD2	72CA	3.379	70	200NE	280D2	3.552
	72CE1	72CZ	1.384		200CZ	280D2	3.594
	72CE1	72CD1	1.398		200NH2	280D2	2.807
30	72CE1	72CE2	2.392		200NH2	28CG	3.947
	72CE1	72CG	2.421		2080	70CE2	3.609
	72CE1	28OD1	2.694	75 .	2080	700H	3.637
	72CE1	72CD2	2.767				
	72CE1	28CG	3.411				
35	72CE1	280D2	3.724				
	72CE1	72CB	3.806				
	72CE2	72CZ	1.381		·		
	72CE2	72CD2	1.396				··
	72CE2	72CE1	2.392				
40	72CE2	72CG	2.420			•	
	72CE2	72CD1	2.769				
	72CE2	72CB	3.802				
	72CZ	72CE2	1.381				

					101A	79NH1	3.816
	Table IIB				101A	31N	3.871
	Interatomic di	stances in	the active	45	102A	79NH2	3.383
	site of UPPS i				102A	280D2	3.815
5	FROM	TO	771411		103A	29N	3.119
	DISTANCE, And				103A	30N	3.133
	1C1	79NH1	3.600		103A	31N	3.539
	1C1	79NH2	3.700	50	103A	29C	3.628
	101	270	3.689		103A	30CB	3.710
10	1C2	300D1	3.734		103A	29CA	3.773
	102	45NE2	3.829		103A	30CA	3.821
	1C2	79NH1.	3.943		1PB	29N	3.332
	1C3	710	3.693	55	1PB	29CA	3.751
	1C4	710	3.205		1PB	29C	3.892
15	1C4	71C	3.901		1PB	30N	3.917
	1C5	710	3.250		1PB	31N	3.953
	1C5	45CD2	3.935		101B	280D2.	3.279
	1C6	300D1	3.590	60	101B	29N	3.303
	1C6	710	3.792		101B	28CG	3.959
20	1C7	710	3.815		103B	29CA	3.054
	1C10	49N	3.149		103B	32N	3.066
	1C10	450	3.182	~ ~	103B	32CB	3.174
·	1C10	48C	3.455	65	103B	29¢ .	3.179
	1C10	48CA	3.529	•	103B	29N	3.239
25	1C10	300D1	3.732		103В	290	3.525
	1C10	49CA	3.898		103B	30N	3.683
	1C11	90CD1	3.926	70	103B	31N	3.695
	1C13	143CE2	3.797	70	103B	32CA	3.724
	1C14	143CE2	3.506		·		
30 .	1C14	143CZ	3.626				
	1C14	143CD2	3.943				
	1C14	91CG	3.966			•	
	1C14	91CA	3.973				
	1C15	49SD	3.501				
35	. 1C15	94CG	3.603				
	1C15	94CB	3.631				
	1C15	94CD1	3.657				• *
	1C15	49CG	3.786				
40	1C15	900	3.878			•	•
40	1PA	79NH2	3.866				
	101A	79NH2	3.513				
	101A	45CE1	3.716				

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	· · · · · · · · · · · · · · · ·	

		1			1017	280D2	3.512
	Table IIC. Inter	ratomic dis	stances in	35	1017	28CG	3.928
	the active site	of UPPS in	n complex		1018	28OD2	2.364
	with IPP		•		1018	28CG	3.315
5	FROM	TO		,	1018	247NH2	3'.318
	DISTANCE, Ang			, ,	1018	280D1	3.896
	1C01	700	3.809	40	1P19	2080G	3.381
	1C02	280D2	3.216		1P19	250CA	3.746
	1C02	270	3.687	·	1P19	206NH1	3.934
10	1C02	28CB	3.980		1P19	2470	3.982
	1C05	710	2.963		1P19	206CD	3.996
	1C05	700	3.179	45	1020	2080G	2.922
	1C05	71C	3.316	1	1020	250N	3.251
	1C05	72N	3.740		1020	250CA	3.346
15	1C05	70C	3.796		1020	217CE2	3.424
	1C05	72CA	3.902		1020	208CB	3.573
•	1C05	76ND2	3.926	50	1020	2470	3.929
	1C09	70CD2	3.339		1021	206NH1	2.419
	1C09	70CE2	3.717		1021	206CD	2.885
20	1C09	70CG	3.726		1021	206CZ	3.136
	1C12	70CE2	3.543	~ ~	1021	206NE	3.301
	1C12	70CD2	3.700	55	1021	2080G	3.619
	1014	200NH2	3.012		1021	200NH2	3.888
	1014	2080G	3.176		1022	250CA	2.964
25	1014	208CB .	, 3.901		1022	247NE	3.080
	1P15	280D2	3.515	60	1022	2470	3.568
	1P15	200NH2	3.785	60	1022	247CZ	3.603
	1016	76ND2	3.221		1022	247CG	3.609
	1016	760D1	3.395	1	1022	250C	3.669
30	1016	76CG	3.703		1022	247CD	3.708
	1016	250CA	3.833	65	1022	250N	3.789
	1016	730G	3.895	0J	1022	247NH2	3.794
	1017	200NH2	3.277		1022	2500	3.945

Table IIIA
Interatomic angle between residues in the active site of the native UPPS

	ATOM1	ATOM2	ATOM3	ANGLE, degree
	27CA	27N	27CB	36.380
75	27CA	27N	27C	34.390

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		27CA	27N	27CG	59.730
		27CA	27N	28N	48.110
		27CA	27N	700	114.81
		27CA	27N	270	41.610
5		27CB	27N	27C	61.060
		27CB	27N	27CG	31.140
	Per .	27CB	27N	28N	81.760
		27CB	. 27N	700	86.200
		27CB	27N	270	55.020
10		27C	, 27N	27CG	90.640
		27C	27N	28N	24.120
		27C	27N ·	700	105.55
		27C	27N	270	18.750
		27CG	27N	28N	107.82
15		27CG	27N	700	86.660
		27CG ,	27N	270	86.150
		28N	27N	700	122.16
		28N	27N	270	41.130
		700	27N	270	87.110
20		27N	27CA	27C	112.36
		27N	27CA	27CB	108.92
		27N	27CA	-270	114.32
	•	2.7N	27CA	. 28N.	104.81
		27N	27CA	27CG	90.350
25	,	27N	27CA ·	28CA	106.75
		27N	27CA	700	45.650
		27C	27CA	27CB	110.35
		27C	27CA	270	26.110
		27C	27CA	28N	29.970
30		27C	27CA	27CG	143.84
		27C	27CA	28CA	21.730
		27C	27CA	700	99.510
		27CB	27CA	270	85.940
		27CB	27CA	28N	137.21
35		27CB	27CA	27CG	33.580
		27CB	27CA	28CA	130.36
		27CB	27CA	700	73.670
		270	27CA	28N	56.090
,		270	27CA	27CG	119.32
40		270	27CA	28CA	47.840
		270	27CA	700	83.930
		28N	27CA	27CG	164.74
		28N	27CA	28CA	8.280
		•			420

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	28N	27CA	700	115.89
	27CG	27CA .	28CA	161.71
	27CG	27CA	700	76.000
	28CA	27CA	700	111.21
5	27CG	27CB	27CA	112.71
	27CG	27CB	27N	93.000
	-27CG	27CB	27C	147.22
	27CG	27CB	270	171.19
	27CG	27CB	27SD	35.510
.10	27CG	27CB	27CE	64.550
	27CG	27CB	28N	136.98
	27CG	27CB	700	91.600
	27CA	27CB	27N	34.700
	27CA	27CB	27C	34.610
15	27CA	27CB	270 :	60.300
	27CA	27CB	27SD	147.93
	27CA	27CB	27CE	148.37
	27CA	27CB	28N	26.360
	27CA	27CB	700	83.880
20	27N	27CB	27C	60.210
	27N	27CB	270	78.260
	27N	27CB	27SD	121.10
	27N	27CB	27CE	114.61
	27N	27CB	28N	57.150
25 .	27N	27CB	700	54.530
	27C	27CB	270	26.560
	27C	27CB	27SD	177.03
	27C	27CB	27CE	141.31
	27C	27CB	28N	11.650
30	27C	27CB	700	87.400
	270	27CB	27SD	150.53
,	270	27CB	27CE	118.05
	270	27CB .	28N	37.710
	270	27CB	700	82.510
35	27SD	27CB	27CE	36.000
·	27SD	27CB	28N	171.28
	27SD .	27CB	700	91.440
	27CE	27CB	28N	152.38
	27CE	27CB	700	65.120
40	28N	27CB	700	93.470
	27CB	27CG	27SD	115.29
	27CB	27CG	27CA	33.710
	27CB	27CG	27CE	86.330
				421

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11 0 00/040/00	104,00

	27CB	27CG	27N	55.860
	27CB	27CG	27C	20.460
	27SD	27CG	27CA	148.72
	27SD	27CG	27CE	40.300
5	27SD	27CG	27N	148.35
	27SD	27CG	27C	135.74
	27CA	27CG	27CE	113.74
	27CA	27CG	27N	29.920
	27CA	27CG	27C	13.340
10	27CE	27CG	27N	108.96
	27CE	27CG	27C	103.84
	27N	27CG	27C	39.820
	27CG	27SD	27CE	100.58
	27CG	27SD	27CB	29.200
15	27CE	27SD	27CB	80.830
	27SD	27CE	27CG	39.120
	27SD	27CE	27CB	63.170
	27SD	27CE	700	112.50
	27SD	27CE	71CA	151.28
20	27SD	27CE	70C	125.18
	27SD	27CE	71N	144.45
	27CG	27CE	27CB	29.120
	27CG	27CE	700	76.540
	27CG	27CE	71CA	112.15
25	27CG	27CE	70C	92.940
	27CG	27CE	71N	110.19
	27CB	27CE	700	66.630
	27CB	27CE	71CA	89.780
	27CB	27CE	70C	84.950
30	27CB	27CE	71N	96.340
	700	27CE	71CA	42.450
	700	27CE	70C	18.330
	700	27CE	71N	33.650
	71CA	27CE	70C	36.360
35	71CA	. 27CE	71N	21.480
	70C	27CE	71N	19.290
	270	27C	28N	123.65
	270	27C	27CA	121.05
	270	27C	28CA	93.890
40	270	27C	27N	120.82
	270	27C	27CB	88.040
	270	27C	28C	92.660
	270	27C	28CB	106.86
				422

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	270	27C	280	106.26
	270	27C	27CG	100.06
	28N	27C	' 27CA	115.29
	28N	. 27C	28CA	29.780
5	28N	∴ 27C	27N	106.14
	28N	27C	27CB	146.02
	28N	27C	28C	37.660
	28N	27C	28CB	22.870
	28N	27C	280	36.990
10	28N	27C	27CG	135.19
	27CA	27C	28CA	145.05
	27CA	27C	27N	33.240
	27CA	27C	27CB	35.040
	27CA	27C	28C	139.44
15	27CA	27C	28CB	129.53
	27CA	27C	280	120.75
	27CA	27C	27CG	22.820
	28CA	27C	27N	128.73
•	28CA	27C	27CB	168.13
20	28CA	27C	28C	24.300
	28CA	27C	28CB	20.290
,	28CA	. 27C	280	39.070
	28CA	, 27C	27CG	163.41
•	27N	27C	27CB"	58.730
25	27N	27C	28C	143.49
	27N	27C	28CB	108.49
	27N	27C	280	132.89
	27N	27C	27CG	49.540
	27CB	27C	28C	143.99
30	27CB .	27C	28CB	164.54
	27CB	27C	280	129.27
	27CB	27C	27CG	12.320
	28C	27C	28CB	41.960
	28C	27C	280	18.970
35	28C	27C	27CG	144.47
	28CB	27C	280	51.260
	28CB	27C	27CG	152.23
	280	27C	27CG	126.78
	27C	270	28N	29.360
40	27C	270	27CA	32.830
	27C	270	27CB	65.400
	27C	270	28CA	60.270
	27C	270	27N	40.420
				423

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	27C	270	72N	119.25
	27C	270	72CA	115.84
	27C	270	28C	67.810
	27C	270	72CB	133.62
5	28N	270	27CA	62.190
	28N	270	27CB	94.090
	28N	270	28CA	30.930
	28N	270	27N	65.570
	28N	270	72N	123.25
10	28N	270	72CA	107.43
	28N	270	28C	41.640
	28N	270	72CB	115.21
	27CA	270	27CB	33.760
	27CA	270	28CA	93.110
15	, 27CA,	270	27N	24.070
	27CA	270	72N	106.33
	27CA	270	72CA	117.49
	27CA	270 [.]	28C	98.190
	27CA	270	72CB	141.08
20	27CB	270	28CA	124.52
	27CB	270	27N	46.720
	27CB	270	72N	98.900
	27CB	270	72CA	120.62
	27CB	270	28C	121.57
25.	27CB	270	72CB	137.19
	28CA	270	27N	93.240
	28CA	270	72N	116.21
	28CA	270	72CA	93.160
	28CA	270	28C	23.060
30	28CA	270	72CB	91.060
	27N	270	72N	84.810
	27N	270	72CA	93.480
	27N	270	28C	106.96
	27N	270	72CB	117.07
35	72N	270	72CA	24.250
	72N	270	28C	134.35
	72N	270	72CB	39.290
	72CA	270	28C	110.11
	72CA	270	72CB	23.590
40	28C	270	72CB	100.52
	27C	28N	28CA	123.27
	27C	28N	270	26.990
	27C	28N	28CB	144.68
				424

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	27C	28N	27CA	34.730
	27C	28N	. 28C	123.32
	27C	28N	1 280	126.47
	27C	28N	27N	49.740
5	27C	28N	28CG	128.18
	27C	28N	. 29N	114.65
	27C	28N	27CB	22.340
	28CA	. 28N	270	96.310
	28CA	28N	28CB	37.450
10	28CA	28N	27CA	157.96
	28CA	28N	28C	35.130
	28CA	28N	280	59.120
	28CA	28N	27N	150.28
	28CA	28N	28CG	32.800
15	28CA	28N	29N	28.800
	28CA	28N	27CB	143.49
	270	28N	28CB	123.25
	270	28N	27CA	61.720
	270	28N	28C	101.36
20	270	28N	280	114.28
	270	28N	27N	73.310
	270	28N	28CG	106.86
	270	28N	29N	90.580
	270	28N	27CB	48.200
25	28CB	28N	27CA	153.91
	28CB	28N	28C	61.510
	28CB	28N	. 280	74.560
	28CB	28N	27N	126.83
	28CB	28N	28CG	16.730
30	28CB	. 28N	29N	62.020
	28CB	28N	27CB	163.11
	27CA	28N	28C	144.55
	27CA	28N	280	129.18
	27CA	28N	27N	27.080
35	27CA	28N	28CG	147.04
	27CA	28N	29N	142.51
	27CA	28N	27CB	16.430
*	28C	28N	280	25.920
	28C	28N	27N	171.56
40	28C	28N	28CG	64.910
	28C	28N	29N	12.790
	28C	28N	27CB	130.53
	280	28N	27N	150.57
				425

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		280	28N	28CG	83.730
		280	28N	. 29N	37.940
		280	28N	27CB	121.55
	•	27N	28N	28CG	122.57
5		27N	28N	29N	163.88
		27N	28N	27CB	41.090
		28CG	28N	29N	61.280
		28CG	28N	27CB	148.65
		29N	28N	27CB	126.52
10		28N	28CA	28CB	107.02
		28N	28CA	28C	112.05
		28N	28CA	. 280	89.640
		28N	28CA	27C	26.940
		28N	28CA	29N	134.67
15		28N	28CA	28CG	128.94
		28N	28CA	270	52.760
		28N	28CA	280D1	152.34
		28N	28CA	280D2	113.57
	•	28N	28CA	27CA	13.760
20		28N	28CA	29CA	127.71
		28N	28CA	72CD1	129.63
		28CB	28CA	28C	109.05
	,	.28CB	28CA	280	105.11
		28CB	28CA	27C	125.81
25	•	28CB	28CA	· 29N	108.67
		28CB	28CA	28CG	32.900
		28CB	28CA	270	139.28
		28CB	28CA	280D1	49.370
		28CB	28CA	280D2	36.310
30		28CB	28CA	27CA	116.48
		28CB	28CA	29CA	108.66
		28CB	28CA	72CD1	91.900
		28C	28CA	280	26.130
		28C	28CA	27C	114.99
35		28C	28CA	29N	28.520
		28C	28CA	28CG	111.90
		28C	28CA	270	111.43
		28C	28CA	28OD1	91.730
		28C	28CA	280D2	129.48
40		28C	28CA	27CA	114.99
		28C	28CA	29CA	18.660
		28C	28CA	72CD1	104.41
		280	28CA	27C	101.07
					426

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	280	28CA	29N	54.660
	280	28CA	28CG	122.89
	280	28CA	270	109.10
	280	28CA	280D1	109.04
5	280	28CA	280D2	138.00
	280	28CA	27CA	96.260
	280	28CA	29CA	44.780
	280	28CA	72CD1	130.51
	27C	28CA	29N	125.15
10	27C	28CA	28CG	133.04
	27C	28CA	270	25.830
	27C	28CA	280D1	149.66
	27C	28CA	280D2	115.49
	27C	28CA	27CA	13.230
15	27C	28CA	29CA	123.17
	27C	28CA	72CD1	105.64
	29N	28CA	28CG	95.780
	29N	28CA	270	108.87
	29N	28CA	280D1	72.600
20	29N	28CA	280D2	111.76
	29N	28CA	27CA	131.70
	29N	28CA	29CA	9.900
	29N	28CA	72CD1	75.920
	28CG	28CA	270°	127.43
25	28CG	28CA	280D1	23.400
•	28CG	28CA	280D2	17.580
	28CG	28CA	27CA	131.69
	28CG	28CA	29CA	101.05
	28CG	28CA	72CD1	59.120
30	270	28CA	280D1	132.28
	270	28CA	280D2	112.81
	270	28CA	27CA	39.060
	270	28CA	29CA	111.06
	270	28CA	72CD1	82.410
35	280D1	28CA	280D2	39.380
	280D1	28CA	27CA	153.28
	280D1	28CA	29CA	78.560
	280D1	28CA	72CD1	50.890
<u></u>	280D2	28CA	27CA	114.54
40	280D2	28CA	29CA	117.93
	280D2	28CA	72CD1	59.590
	27CA	28CA	29CA	127.25
	0500	0000		

27CA

28CA

427

117.24

72CD1

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	29CA	28CA	72CD1	85.820
	28CG	28CB	28CA	113.35
	28CG	28CB	280D2	28.210
	28CG	28CB	280D1	27.410
5	28CG	28CB	28N	135.71
	28CG	28CB	28C	115.15
	28CG	, 28CB	280	133.29
	28CG	28CB	29N	93.780
	28CG	28CB	27C	123.45
- 10	28CA	28CB	280D2	120.99
	28CA	28CB	280D1	101.24
	28CA	28CB	28N	35.530
	28CA	28CB	28C	35.780
	28CA	28CB	280	47.240
15	. 28CA.	28CB	29N	45.280
	28CA	28CB	27C	33.900
	28OD2	28CB	280D1	55.620
	28OD2-	28CB	28N	124.28
	28OD2	28CB	28C	138.72
20	280D2	28CB	280	159.46
	280D2	28CB	29N	118,99
	280D2	28CB	27C	112.73
	280D1	28CB	28N	134.80
	280D1	28CB	28C	90.710
25 .	280D1	28CB	280	106.63
	280D1	28CB	29N	69.220
	280D1	28CB	27C	126.18
	28N	28CB	28C	61.110
	28N	28CB	280	58.660
30	28N	28CB	29N	77.910
	28N	28CB	27C	12.440
	28C	28CB	280	21.080
	28C	28CB	29N	21.570
	28C	28CB	27C	65.640
35	280	28CB	29N	40.530
	280	28CB	27C	67.460
	29N	28CB	27C	79.030
	280D1	28CG	280D2	123.68
.	280D1	28CG	28CB	119.02
40	280D1	28CG	28CA	102.89
	280D1	28CG	72CD1	65.440
	280D1	28CG	28C	81.670
	280D1	28CG	72CE1	45.630
				420

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	280D1	28CG	28N	121.14
	280D1	28CG	29N	61.710
	280D2	28CĠ	· 28CB	117.30
	280D2	, 28CG	28CA	124.73
5	280D2	28CG	72CD1	92.190
	280D2	. 28CG	28C	149.60
	280D2	28CG	72CE1	94.670
	280D2	28CG	28N	108.81
•	280D2	28CG	. 29N	157.61
10	28CB	28CG	28CA	33.750
	28CB	28CG	72CD1	114.38
	28CB	28CG	28C	41.560
	28CB	28CG	72CE1	131.88
	. 28CB	28CG	28N	27.570
15	28CB	28CG	29N	62.520
	28CA	28CG	72CD1	80.800
	28CA	· 28CG	28C	24.870
	28CA	28CG	72CE1	98.780
	28CA	28CG	28N	18.260
20	28CA	28CG	· 29N	41.560
	72CD1	28CG	28C	83.390
	72CD1	28CG	72CE1	23.830
	72CD1	28CG	28N	89.660
	72CD1	28CG	29N	69.760
25	28C	28CG	72CE1	93.160
	28C	28CG	28N	41.390
	28C	28CG	29N	21.080
	72CE1	28CG	28N	111.07
	72CE1	28CG	29N	74.320
30	28N	_ 28CG	29N	59.690
	28CG	280D1	280D2	28.200
	28CG	280D1	28CB	33.570
	28CG	280D1	72CE1	115.15
	28CG	280D1	28CA	53.710
35	. 28CG	280D1	72CD1	92.900
	28CG	280D1	29N	98.940
	28CG	280D1	28C	77.530
	28CG	280D1	72CZ	114.77
46	280D2	280D1	28CB	61.770
40	280D2	280D1	72CE1	98.870
	280D2	280D1	28CA	78.700

280D2

280D2

429

85.680

123.95

72CD1

29N

280D1

280D1

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•	280D2	280D1	28C	104.36
	280D2	280D1	, 72CZ	92.370
	28CB	280D1	72CE1	128.09
	28CB	280D1	28CA	29.390
5	28CB	280D1	72CD1	100.88
	28CB	280D1 .	29N	68.830
	28CB	280D1	28C	46.320
	28CB	280D1	72CZ	137.45
	72CE1	280D1	28CA	104.36
10	72CE1	. 280D1	72CD1	27.220
	72CE1	280D1	29N	91.190
	72CE1	280D1 ·	28C	106.70
	72CE1	280D1	72CZ	17.090
	28CA	280D1	72CD1	78.500
15	28CA	280D1	29N	45.550
	28CA .	280D1	28C	26.560
	28CA	280D1	72CZ	118.77
	72CD1	280D1	29N	78.970
	72CD1	280D1	28C	87.210
20	72CD1	280D1	72CZ	40.290
	. 29N	280D1	28C	22.570
	29N	280D1	72CZ	107.81
	. 28C	280D1	, .72CZ	123.75
	28CG	28OD2	280D1	28.120
25	28CG	280D2	· 28CB	34.490
	28CG	280D2	28CA	37.690
	28CG	280D2	72CD1	67.750
	28CG	280D2	72CE1	65.900
	280D1	280D2	28CB	62.620
30	280D1	280D2	28.CA	61.920
	280D1	280D2	72CD1	57.260
	280D1	280D2	72CE1	45.610
	28CB	280D2	28CA	22.700
	28CB	280D2	72CD1	86.670
35	28CB	280D2	72CE1	94.290
	28CA	280D2	72CD1	66.750
	28CA	280D2	72CE1	79.190
	72CD1	280D2	72CE1	21.880
	280	28C	29N	122.03
40	280	28C	28CA	120.19
	280	28C	29CA	90.290
	280	28C	28N	91.640
	280	28C	28CB	111.86
				430

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	280	28C	27C	96.690
	280	28C	28CG	131.90
	280	28C	280D1	139.06
	280	28C	29C	89.870
5	280	28C	270	110.57
	280	28C	30N	98.730
	29N	28C	28CA	117.78
	29N	28C	29CA	31.750
	29N	28C	28N	142.75
10	29N	28C	28CB	114.75
	29N	28C	27C	128.76
	29N	28C	28CG	91.670
	29N	28C	280D1	71.910
	29N	28C	29C	37.100
15	29N	28C	270	109.27
	29N	28C	30N	42.660
	28CA	28C	29CA	149.50
	28CA	28C	28N	32.820
	28CA	28C	28CB	35.180
20	28CA	28C	27C	40.710
	28CA	28C	28CG	43.230
	28CA	28C	280D1	61.710
	28CA	28C	29C	144.76
	28CA	28C	270	45.510
25	28CA	28C	30N	126.41
	29CA	28C	28N	164.06
	29CA	28C	28CB	135.61
	29CA	28C	27C	145.15
	29CA	28C	28CG	116.00
30	29CA	28C	280D1	95.230
	29CA	28C	29C	20.590
	29CA	28C	270	128.30
	29CA	28C	30N	40.330
	28N	28C	28CB	57.390
35	28N	28C	27C	19.020
	28N	28C	28CG	73.700
	28N	28C	280D1	93.660
	28N	28C	29C	143.57
	28N	. 28C	270	37.000
40	28N	28C	301	123.80
	28CB	28C	27C	72.390
	28CB	28C	. 28CG	23.290
	28CB	28C	280D1	42.970

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	28CB	28C	29C	151.53
	28CB	28C	270	80.610
	28CB	28C	30N	149.41
	. 27C	' 28C	28CG	83.910
5	27C	28C	280D1	101.30
	27C	28C	29C	124.95
	27C	28C	270	19.530
	27C	28C	30N	104.83
	28CG	28C	280D1	20.800
10	28CG	28C	29C	128.73
	28CG	2 ['] 8C	270	84.850
	28CG	28C	30N	127,.77
,	280D1	28C	29C	108.58
	280D1	28C	270	97.440
15	280D1	28C	30N	111.48
	29C	28C	270	109.67
	29C	28C	30N	20.910
	270	28C	30N	88.790
	28C	280	29N	30.260
20	28C	280	28CA	33.680
	28C	280	29CA	62.770
	28C	280	28N	62.440
	28C	280	28CB	47.070
25	28C	280	29C	70.870
25	. 28C	280	, · 27C	64.340
	29N	280	28CA	63.940
	29N	280	· 29CA	32.520
	29N	280	28N	91.600
20	29N	280	28CB	72.570
30	29N	280	29C	42.980
	29N	280	27C	89.830
	28CA	280	29CA	96.440
	28CA	280	28N	31.240
35	28CA	280	28CB	27.650
23	28CA	280	29C	102.81
	28CA	2801	27C	39.860
	29CA	280	28N	123.14
	29CA	280	28CB	101.00
40	29CA 29CA	280	29C	20.550
70		280	27C	117.68
	28N 28N	280	28CB	46.780
		280	29C	121.50
	28N	280	27C	16.540

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	28CB	280	29C	115.55
	28CB	280	27C	61.280
	29C	280	27C	110.43
	28C	29N	29CA	119.54
5	28C	29N	280	27.710
	28C	29N	28CA	33.700
	28C	29N	29C	124.80
	28C	29N	30N	119.21
	28C	29N	28CB	43.680
10	28C	29N	280D1	85.520
	28C	29N	28N	24.470
	28C	29N	290	124.97
	28C	29N	28CG	67.240
	29CA	29N	280	91.840
15	29CA	29N	28CA	153.19
	29CA	29N	29C	30.470
	29CA	29N	30N	57.840
	29CA	29N	28CB	143.85
	29CA	29N	280D1	130.87
20	29CA	29N	28N	140.42
	29CA	29N	290	20.390
	29CA	29N	28CG	145.23
	280	29N	28CA	61.410
	280	29N	29C	100.82
25 .	280	29N	30N	105.29
	280	29N	28CB	66.900
	280	29N	28OD1	105.70
	280	29N	28N	50.460
	280	29N	290	98.780
30	280	29N	28CG	90.190
	28CA	29N	29C	148.72
	28CA	29N	30N	127.48
	28CA	29N	28CB	26.040
	28CA	29N	280D1	61.840
35	28CA	29N	28N	16.530
•	28CA	29N	290	154.26
	28CA	29N	28CG	42.650
	29C	29N	30N	27.380
40	29C	29N	28CB	167.69
40	29C	29N	280D1	148.53
	29C	29N	28N	132.65
	29C	29N	290	10.120
	29C	29N	28CG	167.76
				122

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	30N	29N	28CB	153.45
	30N	29N	280D1	147.27
÷	30N	29N	. 28N	114.75
	3 [.] 0N	29N	290	37.500
5	30N	29N	28CG	153.02
	28CB	29N	280D1	41.940
	28CB	29N	28N	40.060
	.28CB	· 29N	290	162.27
	28CB	29N	28CG	23.710
10	280D1	29N	28N	78.310
	280D1	29N	290	143.62
	280D1	29N	28CG	19.360
	28N	29N	290	137.73
	28N	29N	28CG	59.030
15	290	29N	28CG	162.19
	29N	29CA	29C	120.43
	29N	29CA	290	147.28
	29N	29CA	28C	28.710
	29N	29CA	30N	91.970
20	29N	29CA	280	55.640
	29N	29CA	30CA	102.08
	29N	29CA	28CA	16.910
	29C	29CA	290	, 26.900
	29C	29CA	28C	125.53
25 ⁻	29C	29CA	30N	28.490
	29C	29CA	280	120.71
	29C	29CA	30CA	18.360
	29C	29CA	28CA	125.32
	290	29CA	28C	146.41
30	290	29CA	30N	55.390
	290	29CA	280	129.18
	290	29CA	30CA	45.260
	290	29CA	28CA	150.37
	· 28C	29CA	30N	100.21
35	28C	29CA	280	26.940
	28C	29CA	30CA	109.44
	28C	29CA	28CA	11.840
	30N	29CA	280	105.06
	30N	29CA	30CA	10.130
40	30и	29CA	28CA	97.730
	280	29CA	30CA	111.26
	280	29CA	28CA	38.780
	30CA	29CA	28CA	107.63
	•			434

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		290	•	29C	30N	122.23
		290		29C	29CA	119.22
		290		29C	30CA	90.610
		290		29C	29N	148.27
5		290		29C	30C	72.390
		290		29C	31N	81.660
		290		29C	28C	145.21
		290		29C	30CB	106.09
		290	•	29C	280	128.94
10		290		29C	30ND2	114.58
		290	•	29C	300	59.110
		30N		29C	29CA	118.55
		30N		29C	30CA	31.620
	1	30N		29C	29N	89.480
15		30N		29C	30C	55.670
		30N		29C	. 31N	62.350
		30N	•	29C	28C	88.620
		30N		29C	30CB	16.150
		30N		29C	280	96.860
20		30N		29C	30ND2	34.300
		30N		29Ç	300	65.850
	•	29CA		29C	30CA	150.17
		29CA	,	29C	29N	29.100
	,	29CA	••	29C	30C	154.01
25		29CA	t	29C	, 31N	129.42
		29CA		29C	28C	33.880
		29CA		29C	. 30CB	134.69
		29CA		29C	280	38.750
		29CA		29C	30ND2	114.59
30		29CA	*	29C	300	163.18
		30CA		29C	29N	121.08
	•	30CA		29C	30C	30.880
		30CA		29C	31N	49.750
		30CA		29C	28C	118.92
35		30CA		29C	30CB	15.480
		30CA		29C	280	122.44
		30CA		29C	30ND2	44.530
		30CA		29C	300	36.420
		29N		29C	30C	134.46
40		29N		29C	31N	116.51
		29N		29C	28C	18.100
		29N		29C	30CB	105.61
		29N		29C	280	36.200
						435

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	29N	29C	30ND2	91.810
	29N	29C	300	148.84
	30C	29C	31N	24.920
	30C	29C	28C	142.20
5	30C	29C	30CB	41.950
	30C	29C	280	152.26
	30C	29C	30ND2	75.400
	30C	. 29C	300	14.380
	31N	29C	28C	130.82
10	31N	. 29C	30CB	54.430
	31N	29C	280	149.26
	31N	29C	30ND2	91.600
	31N	29C	300	35.810
	28C	29C	30CB	104.20
15	28C	29C	280	19.260
	28C	29C	30ND2	80.950
	28C	29C	300	154.43
	30CB	29C	280	110.33
	30CB	29C	30ND2	37.220
20	30CB	29C .	300	50.510
	280	29C	30ND2	78.810
	280	29C	300	156.96
	30ND2	. 29C	. , , , 300	78.520
	29C	290	30N	30.100
25	· 29C	290	29CA	33.880
	29C	290	30CA	62.390
	29C	290	30C	83.190
	29C	290	31N	76.100
	29C	290	300	102.69
30	29C	290	32N	109.56
	29C	290	29N	21.600
	29C	290	32C	146.61
	30N	290	29CA	63.980
	30N	290	30CA	32.290
35	30N	290	30C	56.600
	30N	290	31N	58.480
	30N	290	300	74.320
	30N	290	32N	106.90
	30N	290	29N	51.700
40	30N	290	32C	139.48,
	29CA	290	30CA	96.270
	29CA	290	30C	113.67
	29CA	290	31N	98.860
				436

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		29CA	290	300	134.07			
		29CA	290	32N	106.33			٠,
		29CA	290	29N	12.320			
	•	29CA	290	32C	130.82			
	5	30CA	290	30C	31.760			
		30CA	290	31N	47.590			•
		30CA	290	300	44.420			
	•	30CA	290	32N	98.540			
		30CA	290	29N	83.970			
	10	30CA	290	32C	116.67		,	•
		30C	290	31N	24.420			
		30C	290	300	20.410			
		30C ·	290	32N	68.450	,		
		30C	290	29N	102.30		•	
	15	30C	. 290	32C	85.980			•
		31N '	290	300	39.770		•	
		31N	290	32N	51.990			
		31N	290	29N	89.920			
		31N	290	32C	81.050			
	20	300	290	32N	67.440			
		300	290	29N	122.54			
		300	290	32C	72.860		•	
		32N	290	29N	107.39			
		32N	290	32C	37.500			
	25	29N	290	32C	137.88			_
•		29C	30N	30CA	119.61			·
		29C	30N	290	27.670	,		
		29C	30N	30CB	155.13			
		29C	30N	29CA	32.960		•	
	30	29C	30N	30C	97.880			
		29C	30N	30ND2	129.93			
		29C	30N	31N	92.760			
		29C	30N	29N	63.130			
		29C	30N	30CG	154.93			
	35	29C	30N	300	93.970			
		29C	30N	28C	70.460			
		30CA	30N	290	91.950			
		30CA	30N	30CB	35.520			
		. 30CA .	30N	29CA	152.57			••
	40	30CA	30N	30C	34.960			
		30CA	30N	30ND2	70.210			
		30CA	30N	31N	60.460			
		30CA	30N	29N	176.68		•	
					437			
								•

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W O 03/048/33	1 C 17 USV2/30 / 13

	30CA	30N	30CG	57.170
	30CA	30N	300	30.530
	30CA	30N	28C	162.37
	290	30N	30CB	127.47
5	290	30N	29CA	60.630
	290	30N	30C	73.990
	290	30N	30ND2	123.38
	290	30N	31N	78.450
	290	30N	29N	90.800
·10	290	30N	30CG	138.42
	290	30N	300	67.810
	290	30N	28C	97.020
	30CB	30N	29CA	171.88
	30CB	30N	30C	60.600
15	30CB	30N	30ND2	53.970
	30CB	30N	31N	74.000
	30CB	30N	29N	141.69
	30CB	30N	30CG	30.100
	30CB	30N	300	62.310
20	30CB	30N	28C	133.31
	29CA	30N	30C	125.63
	29CA	30N	30ND2	123.82
	29CA	30N .	31N.	109.21
	29CA	30N	29N	30.190
25 ·	29CA	30N	, 30CG	145.25
	29CA	30N	300	125.03
	29CA	30N	28C	39.460
	30C	30N	30ND2	105.12
	30C	30N	31N	28.440
30	30C	30N	29N	144.78
	30C	30N	30CG	88.830
	30C	30N	300	12.250
	30C	30N	28C	162.66
	30ND2	30N	31N	126.86
35	30ND2	30И	29N	109.72
	30ND2	30N	30CG	26.110
	30ND2	30N	300	99.330
	30ND2	30И	28C	92.200
	31N	30N	29N	118.36
40	31N	30N	30CG	103.99
	31N	30N	300	39.730
	31N	30N	28C	136.29
	29N	30N	30CG	121.32
	•			438

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	29N	30N	300	150,40
	29N	30N	28C	18.130
	30CG	30N	4 300	87.520
	30CG	30N	28.C	107.18
5	300	30N	28C	164.36
	30N	30CA	30CB	110.71
	30N	30CA	30C	112.03
	30N	30CA	300	131.50
	30N	30CA	· 29C	28.760
10	30N	30CA	31N	88.380
	30N	30CA	30CG	93.640
	30N	30CA	30ND2	78.770
	30N	30CA	290	55.760
	30N	. 30CA	300D1	97.290
15	30N	30CA	29CA	17.300
	30N	30CA	31CA	96.000
	30CB	30CA	30C	109.05
	30CB	30CA	300	109.06
	30CB	30CA	. 29C	139.47
20	30CB	30CA	31N	104.02
	30CB	30CA	30CG	33.600
	30CB	30CA	30ND2	62.890
	30CB	30CA	290	166.48
	30CB	30CA	300D1	25.650
25	30CB	30CA	29CA	128.00
	30CB	30CA	31CA	105.80
	30C ·	30CA	. 300	26.410
	30C	30CA	29C	95.100
20	30C	30CA	31N	29.210
30	30C	. 30CA	· 30CG	142.26
	30C	30CA	30ND2	168.84
	30C	30CA	290	78.730
	30C	30CA	300D1	134.55
25	30C	30CA	29CA	101.94
35	30C	30CA	31CA	20.100
	300	30CA	29C	106.87
	300	30CA	31N	55.620
	300	30CA	30CG	134.40
40	300	30CA	30ND2	145.73
40	300	30CA	290	82.910
	. 300	30CA	300D1	129.50
	300	30CA	29CA	116.83
	300	30CA	31CA	46.510

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CT	/US02/38715

	29C	30CA	31N	81.430
	29C	30CA	30CG	118.36
	29C	30CA	30ND2	95.920
	29C	30CA	290	27.000
5	29C	30CA	300D1	123.63
	29C	30CA	29CA	11.470
	29C	30CA	31CA	85.860
	31N	30CA	30CG	134.14
	31N	30CA	30ND2	155.92
-10	31N	30CA	290	77.160
	31N	30CA	300D1	126.87
	31N	30CA	29CA	83.830
	31N	30CA	31CA	9.120
	30CG	30CA	30ND2	29.300
15	30CG	30CA	290	138.81
	30CG	30CA	300D1	8.000
	30CG	30CA	29CA	108.76
	30CG	30CA	31CA	138.10
	30ND2	30CA	290	110.79
20	30ND2	30CA	300D1	37.290
	30ND2	30CA	29CA	89.220
	30ND2	30CA	31CA	163.85
	290	30CA	300D1,	145.98
	290	30CA	29CA	38.470
25	290	30CA	31CA	77.550
	300D1	30CA	29CA	113.33
	300D1	30CA	31CA	130.32
	29CA	30CA	31CA	89.710
	30CG	30CB	30CA	112.22
30	30CG	30CB	300D1	26.140
	30CG	30CB	30ND2	29.720
	30CG	30CB	30N	94.860
	30CG	30CB	30C	147.37
	30CG	30CB	31N	152.68
35	30CG	30CB	300	143.17
	30CG	30CB	45CD2	90.510
	30CG	30CB	29C	99.810
	30CA	30CB	300D1	138.33
	30CA	30CB	30ND2	82.530
40	30CA	30CB	30N	33.760
	30CA	30CB	30C	35.600
	30CA	30CB	31N	48.310
	30CA	30CB	300	44.510

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	30CA	30CB	45CD2	156.51
	30CA	30CB	29C	25.040
	300D1	30CB	.30ND2	. 55.860
	300D1	30CB	30N	116.48
5	300D1	30CB	30C	173.05
	300D1	30CB	31N	161.44
	300D1	30CB	300	157.21
	300D1	30CB	45CD2	64.420
	300D1	30CB	29C	123.04
10	30ND2	30CB	30N	69.900
	30ND2	30CB	30C	117.72
	30ND2	- 30CB	31N	126.99
	30ND2	30CB	300	117.84
	30ND2	30CB	45CD2	120.16
15	30ND2	30CB	29C	72.880
	30N	30CB	30°C	60.230
	30N	30CB	31N	58.220
	30И	30CB	300	75.530
	, 30и	30CB	45CD2	143.63
20	· 30N	30CB	- 29C	8.720
	30C	30CB	31N	23.510
	30C	30CB	300	19.910
	30C	30CB.	45CD2	122.11
	30C	30CB	1. F 29C	53.020
25	31N	30CB	300	41.290
	31N	30CB	45CD2	108.35
	31N	30CB	29C	54.210
	300	30CB	45CD2	118.45
	300	30CB	29C	67.300
30	45CD2	30CB	29C	149.57
	300D1	30CG	30ND2	122.71
	300D1	30CG	30CB	121.44
	300D1	30CG	30CA	155.54
~ ~	300D1	30CG	.30N	152.61
35	300D1	, 30CG	30C	141.79
	300D1	30CG	45CD2	54.230
	30ND2	30CG	30CB	115.85
	30ND2	30CG	30CA	81.700
	30ND2	30CG	30N	68.090
40	30ND2	30CG	30C	95.470
•	30ND2	30CG	45CD2	175.41
	30CB	30CG	30CA	34.170
	30CB	30CG	30N	55.040
				441

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W O 05/046755	FC1/USU2/30/13

	30CB	30CG	30C	20.460
	30CB	30CG	.45CD2	67.310
	30CA	30CG	30N	29.190
	30CA	30CG	30C	14.140
5	30CA	30CG	45CD2	101.31
	30N	30CG .	30C	40.220
	30N	30CG	45CD2	112.99
	30C	. 30CG	45CD2	87.760
	30CG	300D1	30ND2	29.660
10	30CG	300D1	30CB	32.420
	30CG	300D1	45CD2	108.68
	30CG	300D1 '	. 30CA	16.460
-	30CG	300D1	45CA	107.38
	30ND2	300D1 _.	30CB	62.080
15	30ND2	300D1	45CD2	138.23
	30ND2 .	300D1	30CA	46.090
	30ND2	300D1	45CA	123.53
	30CB	300D1	45CD2	76.330
	30CB	300D1 .	30CA	16.030
20	30CB	300D1 ·	45CA	86.380
	. 45CD2	300D1	30CA	92.220
	45CD2	300D1	45CA	52.870
	.30CA	300D1	45CA -	97.680
	30CG	30ND2	300D1	27.630
25	30CG	30ND2	30CB	34.430
	30CG	30ND2	30CA	69.000
	30CG	30ND2	. 30И	85.800
	30CG .	30ND2	29C	101.18
	300D1	30ND2	30CB	62.060
30	300D1	30ND2	30CA	96.620
	300D1	30ND2	30N	109.98
	300D1	30ND2	29C	125.74
	30CB	30ND2	30CA	34.590
	30CB	30ND2	30N	56.130
35	30CB	30ND2.	29C	69.900
	30CA	30ND2	30N	31.020
	30CA	30ND2	29C	39.550
	30N	30ND2	29C	15.760
	300	30C	31N	123.08
40	300	30C	30CA	120.03
	300	30C	31CA	92.500
	300	30C	30N	142.51
	300	30C	30CB	116.68
				440

WO 03/048733	PCT/US02/38715
110 00/040/00	101,0502,05.10

	300	30C	290	105.73
	300	30C	29C	128.83
	300	30C	31C	78.390
	300	30C	32N	90.790
5	300	30C	30CG	116.60
	300	30C	310	62.180
	31N	30C	30CA	116.88
	31N	30C	31CA	30.580
	31N	30C	30N	89.840
10	31N	30C	30CB	108.74
	31N	30C	290	93.910
	31N	30C	29C	85.950
	31N	30C	31C	50.540
	31N	30C	32N	51.260
15	31N	30C	30CG.	114.95
	31N	30C	310	64.140
	30CA	30C	31CA	147.46
	30CA	30C	30N	33.020
	30CA	30C	30CB	35.360
20	30CA	30C	290	69.500
	30CA	30C	29C	54.020
	30CA	30C	31C	151.01
	30CA	30C	32N	129.67
	30CA	30C	30CG	23.600
25	30CA	30C	310	161.89
	31CA	30C	30N	118.61
	31CA	30C	30CB	130.91
	31CA	30C	290	104.32
	31CA	30C	29C	107.30
30	31CA	30C	31C	28.450
	31CA	30C.	32N	42.540
	31CA	30C	30CG	140.74
	31CA	30C	310	36.590
	30N	30C	30CB	59.170
35	30N	30C	290	49.410
	30N	30C	29C	26.450
	30N	30C	31C	118.85
	30N	30C	32N	98.490
	30N	30C	30CG	50.950
40	30N	30C	310	133.57
	30CB	30C	290	104.22
	30CB	30C	29C	85.030
	30CB	30C	31C	158.64
				443

	WO 03/048733			
	30CB	30C	32N	152.48
	30CB	30C	30CG	12.170
	30CB	30C	310	162.52
	290	30C	29C	24.420
5	290	30C	31C	84.470
	290	30C	32N	63.960
	290	30C	30CG	93.020
	290	. 30C	310	92.450
	29C	30C	31C	97.110
10	29C	30C	32N	75.660
	29 <u>C</u>	30C	30CG	75.610
	29C	30C	310	109.46
	31C	30C	32N	21.500
	31C	30C	30CG	164.83
15	31C	30C	310	16.550
	32N	30C	30CG	148.93
	32N	30C	310	35.130
	30CG	30C	310	174.51
	30C	300	31N	29.760
20	30C	300	30CA	33.560
	30C	300	31CA	61.240
	30C	300	31C	78.850
,	. 30C	300	30CB	43.410
	30C	300	290	53.850
25.	30C	300	310	99.410
	30C	300	30N	25.240
	30C	300	32N	70.370
	30C	300	29C	36.790
20	31N	300	30CA	63.320
30	31N	300	31CA	31.480
	31N	300	31C	52.400
	31N	300	30CB	68.120
	31N	300	290	66.140
25	31N	300	310	71.660
35	31N	300	30N	52.660
	31N	300	32N	50.450
	31N	300	29C	55.140
	30CA	300	31CA	94.800
40	30CA	300	31C	109.50
40	30CA	300	30CB	26.430
	30CA	300	290	52.670
	30CA	300	310	130.30
	30CA	300	30N	17.970

	WO 03/048733			
	30CA	. 300	32N	96.210
	30CA	300	29C	36.710
	31CA	30Ó	4 31C	29.120
	31CA	, . 300	30CB	96.070
5	31CA	. 300	290	84.670
	31CA	300	310	43.350
	31CA	300	30N	83.140
	31CA	300	32N	39.630
	31CA	. 300	. 29C	80.440
10	31C	300	30CB	120.49
	31C	300	290	76.060
	31C	300	310	20.860
•	31C	300	30N	92'. 960
	. 31C	300	32N	19.020
15	31C	300.	29C	80.980
	30CB	3,00	290	78.960
	30CB	300	310	139.22
	30CB	300	30N	42.160
	30CB	300	32N	113.76
20	30CB	300	29C	62.190
	290	300	310	91.030
	290	300	30N	37.860
	290	300	32N	57.170
	. 290	300	29C	18.190
25	310	300	30N	113.40
	310	300	32N	35.790
	310	300	29C	99.540
	30N	300	32N	78.500
	30n	300	29C	20.180
30	32N	300	.29C	63.760
	30C	31N	31CA	121.54
	30C	31N	300	27.160
	30C	31N	30CA	33.900
	30C	31N	31C	104.99
35	30C	31N	30N	61.710
	30C	31N	32N	107.97
	30C	31N	29C	69.130
	30C	31N	30CB	47.750
	30C	31N	290	61.660
40	30C	31N	310	95.590
	31CA	31N	300	94.380
	31CA	31N	30CA	155.43
	31CA	31N	31C	33.750

	WO 03/048733			
	31CA	31N	30N	163.31
	31CA	31N	32N	55.530
	31CA	31N	29C	138.46
	31CA	31N	30CB	147.89
5	31CA	31N	290	121.80
	31CA	31N	310	32.550
	300	31N	30CA	61.060
	300	31N	31C	81.750
	300	. 31N	30N	87.610
10	300	, 31N	32N	93.250
	300	31N	29C	89.050
	300	31N	30CB	70.590
	300	31N	290	74.090
	300	31N	310	70.250
15	30CA	31N	31C	132.39
	30CA	311	и ок	31.160
	30CA	31N	32N	121.81
	30CA	318	29C	48.820
	30CA	318	30CB	27.660
20	30CA	318	290	55.240
	30CA	31.0	310	127.00
•	31C	311	1 30N	130.99
•		311	32N	26,800
	31C	311	1 29C	106.84
25	31C	311	1 30CB	152.25
	31C	31N	290	88.200
	31C	311	310	14.520
	30N	311	1 32N	107.85
	30N	311		24.880
30	30и	311	30CB	47.780
	30N	311	290	43.070
	30N	311	310	135.94
	32N	311		82.970
	32N	311		149.45
35	32N	· 311	1 290	68.170
	32N	311		40.090
	29C	311		71.370
	29C	311		22.240
	29C	311	310	114.32

31N

31N

31N

31CA

30CB

30CB

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31N

40

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290

310

310

31C

82.270

93.370

140.26

114.05

1 .

	31N	31CA	310	128.25
	31N	31CA	32N	94.940
	31N	31CA	30C	27.880
•	31N	31CA	300	54.140
5	31N	31CA	32CA	100.77
	31N	31CA	30CA	15.440
	.31C	31CA	310	26.710
	31C	31CA	32N	29.160
	31C	31CA	30C	101.61
10	31C	31CA	300	87.840
	31C	31CA	32CA	19.930
	31C	31CA	30CA	107.84
	310	31CA	32N	55.860
	310	31CA ·	30C	105.79
15	310	31CA	300	83.420
	310	31CA	32CA	46.640
	310	31CA	30CA	116.27
	32N	31CA	30C	94.840
	32N	31CA	300	93.650
20	32N	31CA	32CA	9.260
	32N	31CA	30CA	95.310
	30C	31CA	300	26.250
	. 30C	31CA	32CA	96.610
1	30C	31CA	30CA	12.440
25.	300	31CA	32CA	91.250
	300	31CA	30CA	38.700
	32CA	31CA	30CA	98.990
	310	31C	32N	123.15
	310	31C	31CA	119.67
30	310	31C	32CA	92.510
	310	31C	31N	134.95
	310	31C	32C	74.640
	310	31C	300	94.880
	310	31C	30C	117.27
35	310	31C	32CB	108.24
	310	31C	320	61.430
	32N	31C	31CA	117.17
	32N	31C	32CA	30.680
	32N	31C	31N	95.680
40	32N	31C	32C	55.190
	32N	31C	300	111.38
	32N	31C	30C	99.410
	32N	31C	32CB	15.030
				117

	WO 03/048733			
	32N	31C	320	65.220
	31CA	31C ·	32CA	147.82
	31CA	31C	31N	32.200
	31CA	31C	32C	151.85
5	31CA	31C	300	63.040
	31CA	31C	30C	49.950
	31CA	31C	32CB	132.08
	31CA	31C	320	161.58
	32CA	31C	31N	122.49
10	32CA	31C	32C	31.340
	32CA	31C	300	117.61
	32CA	31C	, 30C	117.02
	32CA	31C	32CB	15.750
	32CA	31C	320	36.890
15	31N	31C	32C	120.12
	31N ,	31C	300	45.850
	31N	31C	30C	24.470
	31N	31C	32CB	108.34
	31N	31C	320	132.40
20	32C	31C .	300	93.190
	32C	31C	30C	102.41
	32C	31C	32CB	41.910
	32C	31C	, , , 320 ,, ,	
	300	31C	30C	22.760
25	300	31C	32CB	114.13
	300 .	31C	320	98.730
	30C	31C	32CB	107.45
	30C	31C	320	112.07
	32CB	31C	320	50.690
30	31C	310	32N	29.650
	31C	310	31CA	33.620
	31C	310	32CA	61.210
	31C	310	32C	80.950
	31C	310	320	100.23
35	31C	310	300	64.260
	31C	310	31N	30.520
	31C	310	30C	46.190
	32N	310	31CA	63.270
	32N	310	32CA	31.570
40	32N	310	32C	55.260
	32N	310	320	72.760

310

32N

32N

448

300

31N

80.920

57.120

		WU 03/048/33				PC1/USU2/38/15
•		32N	310	30C	66.230	
		31CA	310	32CA	94.830	
		31CA	310	32C	111.03	
		31CA	310	320	131.02	
	5	31CA	310	300	53.230	*
		31CA	310	31N	19.200	
		31CA	310	30C	37.620	
		32CA	310	32C	31.410	
		32CA	310	320	43.840	
	10	32CA	310	300	99.290	
		32CA	310	31N	86.720	
		32CA	310	30C	90.250	
		32C	310	320	19.990	•
		32C	310	300	87.840	
	15	32C	310	31N	95.500	•
		32C '	310	30C	88.220	
		320	310	300	100.93	
	•	320	310	31N	115.06	
		320	310	30C	105.40	'
	20	300	310	31N	38.090	
		300	310	30C	18.410	
		31N	310	30C	20.270	•
		31C	32N	32CA	121.54	
pc a d	•	31C	32N	310	27.200	
	25	31C	32N	31CA	33.670	
•		31C	32N	32C	98.180	
		31C	32N	32CB	156.92	
	,	31C	32N	31N	57.520	
		31C	32N	32CG	153.52	
	30	31C	32N	290	104.71	*
		31C	32N	320	94.600	
		31C	32N	30C	59.080	
		31C	32N	300	49.600	
		32CA	32N	310	94.370	** .
	35 .	32CA	32N	31CA	155.18	•
	·	32CA	32N	32C	36.320	
		32CA	32N	32CB	35.500	
		32CA	32N	31N	157.09	
		32CA	32N	32CG	48.480	
	40	32CA	32N	290	102.03	
		32CA	32N	320	32.040	
		32CA	32N	30C	136.41	
		32CA	32N	300	122.95	·
					449	
		,				
				•		

	WO 03/048733				PCT/US02/38715
	310	32N	31CA	60.870	
	310	32N	32C	75.320	•
	310	32N	32CB	129.85	
	310	. 32N	31N	82.780	
5	310	32N	32CG	133.06	
	310	32N	290	115.44	
	310	32N	320	69.350	
	310	32N	30C	78.640	
	310	32N	300	63.290	
. 10	31CA	32N	32C	125.80	
	31CA	32N	32CB	168.95	
	31CA	32N	31N	29.530	
	31CA	32N	32CG	151.44	
	31CA	32N	290	88.480	•
15	. 31CA,	32N	320	125.80	
	31CA	32N	30C	42.620	
	31CA	32N	300	46.720	
	32C	32N	32CB	61.170	•
•	32C	32N	31N	122.11	
20	32C	32N	32CG	82.280	
	32C	32N	290	82.700	•
	32C	32N	320	11.910	

30C

300

31N

290

320

30C

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32CG

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290 320

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31N

31N

31N

31N

31N

32CG

32CG

32CG

32CG

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290

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101.56

86.660

25.840

83.900

63.040

131.25

131.78

143.06

129.20

59.840

20.780

36.300

80.410

101.62

147.03

155.75

94.600

47.590

55.390

140.79

450

109.54

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	320	32N	300	92.920
	30C	32N	300	18.840
	32N	32CA	√ 32C	109.35
	32N	, 32ÇA	32CB	111.02
5	32N	32CA	320	129.14
	32N	32CA	31C	27.780
	32N	32CA	32CG	106.55
	32N	32CA	310	54.050
	32N	32CA	. 31CA	15.570
10	32N	32CA	32CD	105.36
	32C	32CA	32CB	109.02
	32C	32CA	320	26.200
	32C	32CA	31C	92.860
	32C	32CA	32CG	136.13
15	32C	32CA.	310	77.720
	32C	32CA	31CA	99.800
	32C	32CA	32CD	127.84
	32CB	32CA	320	109.26
	32CB	32CA	31C	138.74
20	32CB	32CA	32CG	32.450
	32CB	32CA	310	164.98
	32CB	32CA	31CA	126.49
	32CB	32CA	32CD	19.890
	320	" 32CA	31C	.105.54
25	320	32CA	32CG	124.05
	320	32CA	310	82.830
	320	. 32CA	31CA	115.83
	320	32CA	32CD	122.48
	31C	32CA	32CG	129.49
30	31C	32CA	310	26.280
	31C	32CA	31CA	12.250
	31C	32CA	32CD	131.65
	32CG	32CA	310	145.52
	32CG	32CA	31CA	
35	32CG	32CA	32CD	
	310	32CA	31CA	38.530
	310	32CA	32CD	153.77
	31CA	32CA	32CD	120.38
	32CG	32CB	32CA	115.02
40	32CG	32CB	32N	109.57
	32CG	32CB		
	32CG	32CB		
	32CG	32CB	32NE	54.870
				451

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	32CG	32CB	320	130.87
	32CG	32CB	31C	112.55
	32CA	32CB	32N	33.480
	32CA	· 32CB	32C	35.450
5	32CA	32CB	32CD	148.24
	32CA	32CB	32NE	161.45
	32CA	32CB	320	44.220
	32CA	32CB	31C	25.510
	32N	32CB	32C	58.870
10	32N	32CB	32CD	130.02
	32N	32CB	32NE	157.91
	32N	32CB	320	74.310
	32N	32CB	31C	8.050
	32C	32CB	32CD	169.75
15	32C	32CB	32NE	143.17
	32C	32CB	320	19.650
	32C	32CB	31C	51.900
	32CD	32CB	32NE	28.390
	32CD	32CB	320	150.28
20	32CD	32CB	31C	136.44
	32NE	32CB	320	127.38
	32NE	32CB	31C	164.81
	320	32CB	31C	. 66.560
	32CB	32CG	32CD	111.80
25	32CB	32CG	32NE	95.320
	32CB	32CG	32CA	32.520
	32CB	32CG	32N	44.590
	32CB	32CG	32CZ	94.360
	32CB	32CG	32C	22.610
30	32CD	32CG	32NE	32.100
	32CD	32CG	32CA	143.52
	32CD	32CG	32N	135.66
	32CD	32CG	32CZ	25.790
	32CD	32CG	32C	133.10
35	32NE	32CG	32CA	125.96
	32NE	32CG	32N	137.03
	32NE	32CG	32CZ	8.900
	32NE	32CG	32C	110.60
	32CA	32CG	32N	24.970
40	32CA	32CG	32CZ	126.39
	32CA	32CG	32C	16.050
	32N	32CG	32CZ	132.81
	32N	32CG	32C	39.010
				450

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	32CZ		32CG	32C	112.09
	32NE		32CD	32CG	114.11
	32NE		32CD	*32CZ	26.540
	32NE	1 .	32CD	32CB	96.240
5	32NE		32CD	320B	54.560
,	32NE	•	32CD	, 32NH2	16.130
	32NE		32CD	32CA	105.65
				32CZ	138.57
	32CG	·.	32CD	32CB	34.050
10	, 32CG		•	32NH1	159.55
10	32CG	· · ·	32CD	32NH1 32NH2	129.25
	32CG		32CD		23.040
	32CG		32CD	32CA	112.59
	32CZ		32CD	32CB	
15	32CZ		32CD	32NH1 32NH2	28.030 10.410
13	32CZ		32CD	•	
	32CZ	;	32CD	, 32CA	123.99
	32CB		32CD	32NH1	125.78
	32CB		32CD	32NH2	106.62
20	32CB		32CD	32CA	11.860
20	32NH1		32CD	32NH2	38.430
	32NH1		32CD	32CA	137.27
	32NH2		32CD	32CA	117.35
	32CZ		32NE	32CD	124.08
05	32CZ		32NE	32NH1	29.780
25	32CZ	•	32NE	32NH2	29.640
	32CZ		32NE	32CG	154.12
	32CZ		32NE	32CB	139.34
	32CD		32NE	32NH1	94.300
20	32CD		32NE	32NH2	153.72
30	32CD	. '	32NE	32CG	33.790
	32CD		32NE	- 32CB	55.370
	32NH1		32NE	32NH2	59.420
	32NH1		32NE	32CG	125.76
	32NH1		32NE	32CB	124.83
35	32NH2		32NE	32CG	168.08
	32NH2		32NE	32CB	138.50
	32CG		32NE	32CB	29.800
	32NH2		32CZ	32NH1	119.18
	32NH2		32CZ	32NE	120.54
40	32NH2		32CZ	32CD	149.91
	32NH2		32CZ	32CG	135.63
	32NH1		32CZ	32NE	120.28
	32NH1		32CZ	32CD	90.900
					453

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	32NH1	32CZ	32CG	104.70
	32NE	32CZ	, 32CD	29.380
	32NE	32CZ	32CG	16.970
	32CD	32CZ	32CG	15.640
5	32CZ	32NH1	32NH2	30.400
	32CZ	32NH1	. 32NE	29.940
	32CZ	32NH1	32CD	61.070
	32NH2	. 32NH1	32NE	60.340
	32NH2	32NH1	32CD	91.470
10	32NE	, 32NH1	32CD	31.130
	32CZ	32NH2	32NH1	30.420
	32CZ	32NH2	32NE	29.820
	32CZ	32NH2	32CD	19.680
	32NH1	32NH2	32NE	60.240
15	32NH1	32NH2	32CD	50.090
	32NE	32NH2	32CD	10.140
	320	32C	32CA	120.36
	320	32C	32N	143.86
	320	32C	32CB	117.16
20	320	32C .	310	106.87
	320	32C	31C	130.20
	320	32C	32CG	109.42
	. 320	32C.	290	156.25
	32CA	32C	32N	34.330
25	32CA	32C	32CB	35.530
	32CA	. 32C	310	70.870
	32CA	32C	31C	55.810
	32CA	32C	32CG	27.830
	32CA	32C	290	80.940
30	32N	32C	32CB	59.960
	32N	32C	310	49.410
	32N	32C	31C	26.640
	32N	32C	32CG	58.700
	32N	32C	290	59.800
35	32CB	32C	310	105.44
	32CB	32C	31C	86.190
	32CB	32C	32CG	13.640
	32CB	32C	290	73.110
	310	32C	31C	24.410
40	310	32C	32CG	98.470
	310	32C	290	89.350
	31C	32C	32CG	82.980
	31C	32C	290	69.110
				151

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	32CG	32C	290	84.420
	32C	320	32CA	33.440
	32C	320	32CB	43.190
	32C.	320	310	53.140
5	32C	320	32N	24.230
	32C	320	31C	35.710
	32CA	320	32CB	26.510
	32CA	320	310	53.330
	32CA	320	32N	18.820
10	32CA	320	31C	37.570
	32CB	320	310	, 79.570
	32CB	320	32N	42.650
	32CB	320	31C	62.750
	310	320	32N	37.890
15	310	320	31C	18.340
	32N	320	31C	20.180
	45CA	45N	45C	35.410
	45CA	45N	45CB	35.970
	45CA	45N	45CG	57.760
20	45CA	45N	450	31.000
	45CA	45N	45ND1	77.420
	45CA	45N	45CD2	60.650
•	45C	45N	45CB	62.400
	45C	45N	45CG	90.430
25	45C	45N	450	11.620
	45C	45N	45ND1	106.60
	45C	45N	45CD2	96.040
	45CB	45N	45CG	30.090
	45CB	45N	450	63.510
30	45CB	45N	45ND1	44.300
	45CB	45N	45CD2	45.110
	45CG	45N	450	88.630
	45CG	45N	45ND1	21.500
	45CG	45N	45CD2	20.440
35	450	45N	45ND1	107.35
	450	45N	45CD2	90.420
	45ND1	45N	45CD2	34.960
	45N	45CA	45C	110.71
	45N	45CA	45CB	110.04
40	45N	45CA	450	130.63
	45N	45CA	45CG	92.950
	45N	45CA	45CD2	96.020
	45N	45CA	45ND1	79.230
				455

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	45N	45CA	300D1	102.51
	45C	45CA	45CB	112.68
	. 45C	45CA	450	26.040
	45C	45CA	45CG	145.56
5	45C	45CA	45CD2	153.21
	. 45C	45CA	45ND1	144.96
	45C	45CA	300D1	115.68
	45CB	45CA	450	111.13
	45CB	45CA	45CG	33.260
10	45CB	45CA	45CD2	53.130
	45CB	45CA	45ND1	36.450
	45CB	45CA	300D1	104.60
	450	45CA	45CG	136.10
	450	45CA	45CD2	130.56
15	450	45CA	45ND1	147.24
	450	45CA	300D1	92.340
	45CG	45CA	45CD2	23.730
	45CG	45CA	45ND1	16.650
	45CG	45CA	300D1	81.150
20	45CD2	45CA	45ND1	36.970
	45CD2	45CA	300D1	57.490
	45ND1	45CA	300D1	93.340
	45CG	45CB	45CA	112.60
	45CG	45CB	45N	94.770
25 ⁻	45CG	45CB	45ND1	27.280
	45CG	45CB	45C	145.67
	45CG	45CB	45CD2	23.270
	45CG	45CB	450	142.79
	45CG	45CB	45CE1	13.750
30	45CG	45CB	45NE2	7.790
	45CA	45CB	45N	
	45CA	45CB	45ND1	
	45CA	45CB	45C	33.450
	45CA	45CB	45CD2	98.710
35	45CA	45CB	450	42.910
	45CA	45CB	45CE1	116.52
	45CA	45CB	45NE2	106.57
	45N	45CB	45ND1	93.090
	45N	45CB	45C	
40	45N	45CB	45CD2	92.950
	45N	45CB	450	74.290
	45N	45CB	45CE1	92.170
	45N	45CB	45NE2	92.100
				156

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	45ND1	45CB	45C	151.55
	45ND1	45CB.	45CD2	50.470
	45ND1	. 45CB	450	164.62
	45ND1	45CB	45CE1	13.790
5	45ND1	45CB	45NE2	34.610
	45C	45CB	45CD2	127.91
	45C	45CB	450	19.560
	45C	45CB	45CE1	149.49
	45C	45CB	45NE2	138.98
10	45CD2	45CB	450	120.15
	45CD2	45CB	45CE1	36.740
	45CD2	45CB	45NE2	15.920
	450	45CB	45CE1	153.86
	450	45CB	45NE2	135.00
15	45CE1	45CB	45NE2	20.840
	45CD2	45CG	45ND1	106.01
	45CD2	45CG	45CB	130.89
	45CD2	45CG	45NE2	36.670
	45CD2	45CG	45CE1	71.600
20	45CD2	, 45CG	45CA	107.89
•	45CD2	45CG	45N	109.57
	45CD2	45CG	45C	115.29
	45ND1	45CG	45CB	122.88
	45ND1	45CG	45NE2	69.340
25	45ND1	45CG	45CE1	34.420
	45ND1	45CG	45CA	131.79
	45ND1	45CG	45N	106.27
	45ND1	45CG	45C	132.76
	45CB	45CG	45NE2	166.91
30	45CB	45CG	45CE1	156.97
	45CB	45CG	45CA	34.140
	45CB	45CG	45N	55.140
	· 45CB	45CG	45C	21.710
	45NE2	45CG	45CE1	34.920
35	45NE2	45CG	45CA	135.17
	45NE2	45CG	45N	119.59
	45NE2	45CG	45C	146.62
	45CE1	45CG	45CA	146.63
	45CE1	45CG	45N	117.91
40	45CE1	45CG	45C	156.80
	45CA	45CG	45N	29.290
	45CA	45CG	45C	12.800
	45N	45CG	45C	39.250
				457

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	45CG	45CD2	45NE2	107.24
	45CG	45CD2	45ND1	37.350
	45CG	45CD2	45CE1	72.490
	45CG	45CD2	45CB	25.840
5	45CG	45CD2	45CA	48.370
	45CG	45CD2	300D1	117.87
	45CG	45CD2	30CB	117.20
	· 45CG	. 45CD2	45N	49.990
	45CG	45CD2	30CG	120.03
10	45NE2	45CD2	45ND1	69.890
	45NE2	45CD2	45CE1	34.750
	45NE2	45CD2	, 45CB	13290
	45NE2	45CD2	45CA	141.09
	45NE2	45CD2	300D1	126.04
15	45NE2	45CD2	30CB	94.760
	45NE2 ,	45CD2	45N	118.90
	45NE2	45CD2	30CG	112.54
	45ND1	45CD2	45CE1	35.150
	45ND1	45CD2	45CB	63.110
20	45ND1	45CD2	45CA	81.050
	45ND1	45CD2	300D1	146.78
	45ND1	45CD2	30CB	120.56
	45ND1	45CD2	, , , 45N, .	71.340
	45ND1	45CD2	30CG	137.77
25	45CE1	45CD2	45CB	98.210
	45CE1	45CD2	45CA	112.51
	45CE1	45CD2	300D1	150.32
	45CE1	45CD2	30CB	111.11
	45CE1	45CD2	45N	95.890
30	45CE1	45CD2	30CG	133.23
	45CB	45CD2	45CA	28.160
	45CB	45CD2	300D1	94.020
	45CB	45CD2	30CB	105.83
	45CB	45CD2	45N	41.950
35	45CB	45CD2	30CG	100.29
	45CA	45CD2	300D1	69.640
	45CA	45CD2	30CB	77.970
	45CA	45CD2	45N	23.330
	45CA	45CD2	30CG	72.900
40	300D1	45CD2	30CB	39.260
	300D1	45CD2	45N	75.610
	· 300D1	45CD2	30CG	17.090
	30CB	45CD2	45N	67.700
				450

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	30CB	45CD2	30CG	22.180
	45N	45CD2	30CG	71.680
	45CE1	45ND1	45CG	109.46
•	45CE1	45ND1	45NE2	35.790
5	45CE1	45ND1	45CD2	72.830
	45CE1	45ND1	45CB	139.12
	45CE1	45ND1	45CA	128.17
	45CE1	45ND1	45N	121.97
	45CG	45ND1	45NE2	73.670
10	45CG	45ND1	45CD2	36.640
	45CG	45ND1	45CB	29.840
	45CG	45ND1	45CA	31.560
	45CG	45ND1	45N	52.230
	45NE2	45ND1	45CD2	37.030
15	45NE2	45ND1	45CB	103.39
	45NE2	45ND1	45CA	95.840
	45NE2	45ND1	45N	99.290
	45CD2	45ND1	45CB	66.410
	4.5CD2	45ND1	45CA	61.990
20	45CD2	45ND1	45N	73.700
	45CB	45ND1	45CA	21.110
	45CB	45ND1	45N	42.610
	45CA	45ND1	45N	23.350
	45NE2	45CE1	45ND1	108.40
25	45NE2	45CE1	45CD2	36.370°
	45NE2	45CE1	45CG	72.280
	45NE2	45CE1	45CB	81.380
	45ND1	45CE1	45CD2	72.030
	45ND1	45CE1	45CG	36.120
30	45ND1	45CE1	45CB	27.090
	45CD2	45CE1	45CG	35.910
	45CD2	45CE1	45CB	45.040
	45CG	45CE1	45CB	9.280
	45CE1	45NE2	45CD2	108.88
35	45CE1	45NE2	45ND1	35.810
	45CE1	45NE2	45CG	72.800
	45CE1	45NE2	45CB	77.770
	45CD2	45NE2	45ND1	73.070
1.0	45CD2	45NE2	45CG	36.090
40	45CD2	45NE2	45CB	31.180
	45ND1	45NE2	45CG	36.990
	45ND1	45NE2	45CB	42.000
	45CG	45NE2	45CB	5.290

			•	
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	450	45C	45CA	120.88
	450	45C	45N	144.55
	450	45C	45CB	116.29
	450	45C	48N	59.440
5	450	45C	45CG	116.81
	45CA	45C	45N	33.880
	45CA	45C	45CB	33.870
	45CA	. 45C	48N	105.56
	45CA	45C	45CG	21.630
10	45N	, 45C	45CB	58.880
	45N	45C	48N	97.930
	45N	45C	45CG	50.330
	45CB	45C	48N	135.29
	45CB	45C	45CG	12.620
15	48N	45C	45CG	123.54
	45C	450	45CA	33.070
	45C	450	49N	151.39
	45C	450	48N	100.94
	. 45C	450	45CB	44.150
20	45C	450	45N	23.830
	45C	450	48CA	117.88
	45C	450	48C	140.93
	, 45C	450	, .49CB, .	145.57
	45C	450	49CA	159.39
25	45CA	450	· 49N	146.88
	45CA	450	48N	99.460
	45CA	450	45CB	25.960
	45CA	450	45N	18.370
	45CA	450	48CA	104.05
30	45CA	450	48C	127.00
	45CA	450	49CB	171.68
	45CA	450	49CA	163.08
	4 9 N	450	48N	53.030
	49N	450	45CB	157.31
35	49N	450	45N	139.95
	49N	450	48CA	43.090
	49N	450	48C	19.950
	49N	450	49CB	40.320
40	49N	450	49CA	18.350
40	48N	450	45CB	124.49
	48N	450	45N	87.380
	48N	450	48CA	24.280
	48N	450	48C	40.620

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	48N	450	49CB	88.850
	48N	450	49CA	70.540
	45CB	450	45N	42.200
	45CB	450	48CA	123.39
5	45CB	450	48C	141.10
	45CB	450	49CB	145.86
	45CB	450	49CA	155.67
	45N	450	48CA	98.390
	45N	450	48C	122.61
10	45N	450	49CB	165.95
•	45N	450	49CA	157.92
	48CA	450	48C	24.220
	48CA	450	49CB	83.390
	48CA	450	49CA	61.180
15	48C	450	49CB	59.910
	48C	450	49CA	37.310
	49CB	450	49CA	22.740
	48CA	48N	48C	36.480
	48CA	48N	49N	63.070
20	48CA	48N	450	93.220
	48CA	48N	480	32.330
	48CA	48N	45C	107.30
	48C	48N	49N	29.480
•	48C	48N	450	81.700
25	48C	48N	480	12.410
	48C	48N	45C	101.11
	49N	48N	450	60.320
	4 9 N	48N	480	40.670
	4 9 N	48N	. 45C	79.480
30	450	48N	480	93.900
	450	48N	45C	19.610
	480	48N	45C	113.14
	48N	48CA	48C	108.79
	48N	48CA	480	128.65
35	48N	48CA	· 49N	84.880
	48N	48CA	450	62.500
	48N	48CA	49CA	92.330
,	48C	48CA	480	26.840
40	48C	48CA	49N	29.300
40	48C	48CA	450	83.150
	48C	48CA	49CA	19.890
	480	48CA	49N	56.140
	480	48CA	450	108.36
				4.71

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			,	
	480	48CA	49CA	46.710
	49N	48CA	450	56.090
	49N	48CA	49CA	9.430
	450	48CA	49CA	64.890
5	480	48C	49N	123.25
	480	48C	48CA	119.60
	480	48C	48N	142.82
	480	48C	49CA	92.400
	480	48C	49C	77.160
10	480	48C	450	158.07
	480	48C	49CB	107.61
	480	48C	490	62.950
	49N	48C	48CA	117.14
	49n	48C	48N	88.270
15	49N	48C	49CA	30.850
	49N	48C	49C	52.700
•	49N	48C	450	48.910
	4 9 N	48C	49CB	15.740
	49N	48C	490	64.070
20	48CA	48C	48N	34.730
	48CA	48C	49CA	147.97
	48CA	48C	49C	149.29
,	48CA	48C	450	72.630
	48CA	48C	49CB	132.78
25 ·	48CA	48C	490	158.92
	48N	48C	49CA	116.79
	48N	48C	49C	116.29
	48N	48C	450	57.670
	48N	48C	49CB	103.52
30	48N	48C	490	129.63
	49CA	48C	49C	30.400
	49CA	48C	450	77.590
	49CA	48C	49CB	15.360
•	49CA	48C	490	36.590
35	49C	48C	450	101.29
	49C	48C	49CB	41.610
	49C	48C	490	14.690
	450	48C	49CB	62.570
	450	48C	490	112.91
40	49CB	48C	490	50.700
	48C	480	49N	29.620
	48C	480	48CA	33.560
	48C	480	49CA	61.300
				462

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		48C	480	52N	152.10
		48C	480	49C	79.110
		48C	480	48N	24.770
		48C	480	490	98.710
5		48C	480	52CB	144.86
		48C	480	52CA	158.77
		49N	480	48CA	63.180
		49N	480	49CA	31.680
		49N	480	52N	131.03
10		49N	480	49C	53.300
		49N	480	48N	51.490
		49N	480	490	71.410
		49N	480	52CB	117.10
		49N	480	52CA	129.65
15		48CA	480·	49CA	94.860
		48CA	480	52N	149.04
		48CA	480	49C	108.83
		48CA	480	48N	19.010
		48CA	480	490	128.77
20	•	48CA	480	52CB	165.82
		48CA	480	52CA	165.56
		49CA	480	52N	102.95
		49CA	480	49C	30.500
	•	49CA	480	48N	81.880
25		49CA	480	490	43.260
		49CA	480	52CB	86.590
		49CA	480	52CA	98.140
		52N	480	49C	77.730
		52N	480	48N	140.98
30		52N	480	490	60.200
		52N	480	52CB	42.620
		52N	480	52CA	19.450
		49C	480	48N	90.800
		49C	480	490	20.000
35		49C	480	52CB	79.260
		49C	480	52CA	80.050
		48N	480	490	110.46
		48N	480	52CB	168.46
		48N	480	52CA	159.96
40		490	480	52CB	60.150
		490	480	52CA	60.240
	i	52CB	480	52CA	23.440
		48C	49N	49CA	121.24
					463

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	48C	49N	480	27.130
	48C	49N	48CA	33.560
	48C	49N	49C	101.49
	48C	. 49N	4 9CB	155.88
5	48C	49N	48N	62.250
	48C	49N	450	111.14
	48C	49N	49CG	146.47
	48C	· 49N	490	95.860
	49CA	49N	480	94.120
10	49CA	49N	48CA	154.78
	49CA	49N	49C	36.270
	49CA	49N	49CB	34.930
	4 9CA	49N	48N	160.92
	49CA	49N	450	122.27
15	49CA	49N	49CG	45.130
	49CA	. 49N	490	32.710
	480	49N	48CA	60.680
	480	49N	49C	78.740
	480	49N	49CB	128.86
20	480	49N	48N	87.840
	480	49N	450	134.73
	480	4 9 N	49CG	126.47
	. 480 .	49N	490	70.850
	48CA	49N	49C	127.76
25	48CA	49N	49CB	170,15
	48CA	49N	48N	32.050
	48CA	49N	450	80.820
	48CA	49N	49CG	151.39
	48CA	49N	490	126.10
30	49C	49N	49CB	60.860
	49C	49N	48N	126.57
	49C	49N	450	146.51
	. 49C	49N	49CG	79.150
	49C	49N	490	12.200
35	49CB	49N	48N	140.85
	49CB	49N	450	89.520
	4 9CB	49N	49CG	23.940
	4 9CB	49N	490	63.430
	48N	49N	450	66.650
40	48N	49N	49CG	142.91
	48N	. 49N	490	133.25
	450	49N	49CG	77.820
	450	49N	490	152.81
	•			464

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	4000		400	
	49CG	49N	490	77.780
	49N	49CA	49C	109.24
	4 9 N	49CA	49CB	111.98
~	4 9N	49CA	490	128.08
5	4 9 N	49CA	48C	27.910
	4 9N	49CA	4 9CG	111.32
•	4 9N	49CA	480	54.200
	4 9N	49CA	48CA	15.790
	4 9N	49CA	450	3,9.390
10	4 9C	49CA	49CB	109.06
	4 9C	49CA	490	26.050
	49C	49CA	48C	95.730
	4 9C	49CA	49CG	132.71
	49C	49CA	480	82.190
15	49C	49CA	48CA	101.41
	49C	49CA	450	137.56
	49CB	49CA	490	109.97
	49CB	49CA	48C	139.72
	4.9CB	49CA	4 9CG	31.740
20	49CB	49CA	480	165.37
	49CB	49CA	48CA	127.74
	49CB	49CA	450	75.350
	490	49CA	48C	106.16
•	490	49CA	49CG	120.47
25	490	49CA	480	84.290
	490	49CA	48CA	115.68
	490	49CA	450	163.33
	48C	49CA	49CG	131.14
	48C	49CA	480	26.290
30	48C	49CA	48CA	12.140
	48C	49CA	450	65.100
	4 9CG	49CA	480	142.54
	4 9CG	49CA	48CA	123.44
	49CG	49CA	450	72.630
35	480	49CA	48CA	38.430
	480	49CA	450	90.040
	48CA	49CA	450	53.930
	49CG	49CB	49CA	116.24
•	4 9CG	49CB	4 9 N	114.58
40	49CG	49CB	49C	141.15
	49CG	49CB	49SD	36.600
	49CG	49CB	490	126.24
	49CG	49CB	49CE	53.680
				165

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(

	49CG	49CB	48C	114.27
	49CG	49CB	450	85.220
	49CA	49CB	49n	33.090
	49CA	4 9CB	49C	35.390
5	49CA	49CB	49SD	148.81
	49CA	49CB	490	43.790
	49CA	49CB	49CE	162.24
	49CA	49CB	48C	24.910
	49CA	49CB	450	81.910
10	4 9N	49CB	49C	58.660
	49N	49CB	49SD	148.76
	4 9 N	49CB	490	73.620
	4 9 N	49CB	49CE	132.71
	49N	49CB	48C	8.380
15	4 9N	49CB	450	50.170
	49C	49CB	49SD	147.78
	49C	49CB	490	19.360
	4 9C	49CB	49CE	161.28
	49C	49CB	48C	53.120
20	49C	49CB	450	107.23
	49SD	49CB	490	129.07
	49SD	49CB	49CE	31.240
	49SD	49CB	48C	150.42
	49SD	49CB	450	104.41
25	490	49CB	49CE	153.30
	490	49CB	48C	66.660
	490	49CB	450	123.72
	49CE	49CB	48C	139.97
	49CE	49CB	450	82.570
30	48C	49CB	450	57.520
	49CB	49CG	49SD	113.95
	49CB	49CG	49CA	32.020
	49CB	49CG	49CE	99.440
	49CB	49CG	49N	41.480
35	49CB	49CG	49C	24.300
	49SD	49CG	49CA	142.90
	49SD	49CG	49CE	38.850
	49SD	49CG	49N	152.35
40	49SD	49CG	49C	126.30
40	49CA	49CG	49CE	129.70
	49CA	49CG	49N	23.540
	49CA	49CG	49C	17.180
	49CE	49CG	49N	120.53
	•			466

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	49CE	1:,49CG	49C	122.67		
	49N	49CG	49C	39.050	· ·	•
	49CE	49SD	49CG	98.910	• •	1
	4 9CE	49SD	49CB	90.350	٠	,
5	49CG	. 49SD	49CB	29.450	•	1
	49SD	49CE	. 49CG	42.240	1	
	49SD	49CE	49CB	58.410		
	49CG	. 49CE	49CB	26.880	. *	
	490	49C	4 9CA	120.82		
10	490	49C	49N	142.98		
	490	49C	49CB	118.34	•	•
	490	49C	480	103.81		
	490	49C	48C	126.98		
	490	49C	.52N	58.820		
15	490	49C	4 9CG	107.87		
	49CA	49C	49N	34.490		
	49CA	49C	49CB	35.550		
	49CA	49C	480	67.310		
	49CA	49C	48C	53.870	-	
20	49CA	49C	52N	110.05		•
	49CA	49C	4 9CG	30.110		
	49N	49C	4 9CB	60.480		
	49N	49C	480	47.960		
	49N	49C	48C	25.810	Administration of the second	the London
25	. 49N	49C	52N	98.720		
	49N	49C	49CG	61.800		
	49CB	49C	480	102.42	20	
	49CB	49C	48C,	85.270	•	
	49CB	49C	52N	142.85		
30	49CB	49C	4 9CG	14.550		
	480	49C	48C	23.740		
	480	49C	52N	50.760		
	480	49C	4 9CG	96.450		
	48C	49C	52N	73.810		
35	48C	49C	4 9CG	83.800		
	52N	49C	49CG	129.66	•	
	49C	490	49CA	33.120		
	49C	490	4 9CB	42.300		
	49C	490	52N	102.39		
40	49C	490	480	56.180		
	49C	490	49N	24.820		
	49C	490	52CB	115.92		
	49C	490	52CA	120.50		
			•	467		

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	49C	490	52C	141.89
	49C	490	48C	38.330
	49CA	490	49CB	26.240
	49CA	4 90	52N	103.66
5	49CA	490	480	52.450
	49CA	490	49N	19.220
	49CA	490	52CB	94.190
	49CA	490	52CA	110.37
	49CA	490	52C	132.79
10	49CA	490	48C	37.250
	49CB	490	52N	129.79
	49CB	490	480	78.650
	49CB	490	4 9 N	42.950
	49CB	490	52CB	111.70
15	49CB	490	52CA	132.78
	49CB	490	52C	150.79
•	49CB	490	48C	62.640
	' 52N	490	480	51.750
	52N	490	49N	89.230
20	52N	490	52CB	42.290
	52N	490	52CA	23.070
	52N	490	52C	39.550
	52N	490	48C	, 69.220
	480	490	49N	37.740
25·	480	490	52CB	62.180
	480	490	52CA	64.870
	480	490	52C	87.820
	. 480	490	48C	18.340
	49N	490	52CB	92.020
30	4 9 N	490	52CA	101.56
	49N	490	52C	124.93
	49N	490	48C	20.070
	52CB	490	52CA	24.340
	52CB	490	52C	39.750
35	52CB	490	48C	78.350
	52CA	490	52C	23.400
	52CA	490	48C	83.190
	52C	490	48C	106.15
	52CA	52N	52C	36.160
40	52CA	52N	52CB	35.020
	52CA	52N	480	118.11
	52CA	52N	490	95.590
	52CA	52N	520	34.260
				168

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	52CA	52N	49C	110.60
	52CA	52N	52CG	22.800
	52C	52N	52CB	61.280
	52C	52N	480	138.59
5	. 52C	52N	490	81.420
	52C	52N	520	13.660
	52C	52N	49C	100.20
	52C	52N	52CG	52.160
	52CB	52N	480	83.850
10	52CB	52N	490	75.680
	52CB	52N	520	65.820
	52CB	52N	49C	84.150
	52CB	52N	52CG	12.280
	480	52N	490	68.050
15	480	52N	520	148.48
	480	52N	49C	51.510
	480	52N	52CG	95.630
	490	52N	520	95.050
	490	52N	49C	18.790
20	490	52N	52CG	83.320
	520	52N	49C	113.83
	520	52N	52CG	54.830
	49C	· 52N	52CG	94.170
	52N	52CA	52C	109.25
25	52N	52CA	52CB	112.09
	52N	52CA	520	125.56
	52N	52CA	, 52CG	144.63
	52N	52CA	52CD1	150.46
	52N	52CA	490	61.340
30	52N	52CA	480	42.440
	52N	52CA	52CD2	131.15
	52C	52CA	52CB	110.05
	52C	52CA	520	26.420
	52C	52CA	52CG	92.510
35	52C	52CA	52CD1	100.27
	52C	52CA	490	80.610
	52C	52CA	480	134.08
	52C	52CA	52CD2	101.02
	52CB	52CA	520	113.90
40	52CB	52CA	52CG	32.610
	52CB	52CA	52CD1	56.390
	52CB	52CA	490	73.420
	52CB	52CA	480	70.630
				460

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	52CB	52CA	52CD2	19.210		·
	520	52CA	, 52CG	85.830		
	520	52CA	52CD1	81.620		,
	520	52CA	490	106.77		1
5	520	52CA	480	160.23		
	520	52CA	52CD2	98.070		
	52CG	52CA	52CD1	30.440		
	52CG	52CA	490	96.880		
	52CG	52CA	480	102.57	,	
10	52CG	52CA	52CD2	13.480		
	52CD1	52CA	490	127.05		
•	52CD1	52CA	. 480	114.61	•	
	52CD1	52CA	52CD2	39.470		
	490	52CA	480	54.890		
15	490	·· 52CA	52CD2	87.930		
	480	52CA	52CD2	89.170	•	
	52CA	. 52CB	52CG	114.81	1	
	52CA	52CB	52N	32.900	•	
	52CA	52CB	52C	34.650		
20	52CA	52CB ·	52CD1	92.870		,
	. 52CA	52CB	52CD2	149.21		
	52CA	52CB	520	40.980		
	. 52CA	52CB	490 -	82.240	Office of the second	t in the discount
	52CA	52CB	480	85.930	•	
25	52CG	52CB	52N	147.64	•	
	52CG	52CB	52C	95.470	•	
	52CG	52CB	52CD1	34.840		
	52CG	52CB	52CD2	34.490	•	
	52CG	52CB	520	79.430		
30	52CG	52CB	490	133.14		
	52CG	52CB	480	156.22	•	•
	52N	52CB	52C	58.130	·.	
	52N	52CB	52CD1	120.49		
	52N	52CB	52CD2	176.02		
35	52N	52CB	520	71.010		
	52N	52CB	490	62.030		
	52N	52CB	480	53.530		
	52C	52CB	52CD1	91.890		
	52C	52CB	52CD2	125.58		
40	52C	52CB	520	18.270		
	52C	52CB	490	74.080		
	52C	52CB	480	108.30		
	52CD1	52CB	52CD2	59.460		
	•			470		

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	52CD1	52CB	520	73.720
	52CD1	52CB	490	161.73
	52CD1	52CB	480	139.85
	52CD2	52CB	520	112.23
5	52CD2	52CB	490	119.44
	52CD2	52CB	480	123.55
	520	52CB	490	91.500
	520	52CB	480	123.93
	490	52CB	480	57.670
10	52CD1	52CG	52CD2	109.75
	52CD1	52CG	52CB	109.89
	52CD1	52CG	52CA	89.960
	52CD1	52CG	52C	97.850
	52CD1	52CG	520	83.370
15	. 52CD1 ,	52CG	52N :	97.080
•	52CD2	52CG	52CB	110.66
	52CD2	52CG	52CA	143.17
	52CD2	52CG	52C	152.23
	52CD2	52CG	520	162.30
20	52CD2	52CG	52N	130.60
	52CB	52CG	52CA	32.590
	52CB	52CG	52C	54.470
•	52CB	52CG	520	74.040
	52CB	52CG	52N	20.080
25 -	52CA	52CG	52C	29.630
	52CA	52CG	520	44.400
	52CA	52CG	52N	12.570
	52C	52CG	520	21.080
	52C	52CG	52N	38.700
30	520	52CG	52N	55.970
	52CG	52CD1	52CD2	35.160
	52CG	52CD1	52CB	35.270
	52CG	52CD1	52CA	59.600
	52CG	52CD1	520	71.410
35	52CG	52CD1	52C	57.360
	52CD2	52CD1	52CB	60.550
	52CD2	52CD1	52CA	90.490
	52CD2	52CD1	520	105.83
	52CD2	52CD1	52C	92.480
40	52CB	52CD1	52CA	30.740
	52CB	52CD1	520	
	52CB	52CD1	52C	43.990
	52CA	52CD1	520	
				471

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.1/	USU2/38/

	52CA	52CD1	52C	24.450
	520	52CD1	52C	19.680
	52CG	52CD2	52CD1	35.090
	52CG	52CD2	52CB	34.850
5	52CG	52CD2	52CA	23.350
	52CD1	52CD2	52CB	59.990
	52CD1	52CD2	52CA	50.040
	52CB	52CD2	52CA	11.580
	520	52C	52CA	120.16
10	520	52C	52N	138.43
	520	52C	52CB	121.83
	520	52C	52CG	94.760
	520	52C	52CD1	77.910
	520	52C	490	162.23
15	52CA	52C	52N	34.590
	52CA	52C	52CB	35.300
•	52CA	52C	52CG	57.870
	52CA	52C	52CD1	55.280
	52CA	52C	490	75.990
20	52N	52C	52CB	60.600
	52N	52C	52CG	89.150
	52N	52C	52CD1	89.870
	52N	52C	490	59.020
	52CB	52C	52CG	30.060
25	52CB	52C [']	52CD1	44.120
	52CB	52C	490	66.170
	52CG	52C	52CD1	24.790
·	52CG	52C	490	88.000
	52CD1	52C	490	109.46
30	52C	520	52CA	33.420
	52C	520	52CB	39.900
	52C	520	52CG	64.160
	52C	520	52N	27.900
•	52C	520	52CD1	82.410
35	52CA	520	52CB	25.130
	52CA	520	52CG	49.770
	52CA	520	52N	20.180
	52CA	520	52CD1	56.910
	52CB	520	52CG	26.530
40	52CB	520	52N	43.170
	52CB	520	52CD1	42.670
	52CG	520	52N	69.200
	52CG	520	52CD1	25.220

	52N	520	52CD1	76.680
	70CA	70N	70CB	37.460
	70CA	70N	, 40C	35.750
	70CA	70N	700	55.180
5	.70CA	70N	71N	35.970
	70CA	70N	70CG	27.370
	70CB	70N	70C	62.020
	70CB	· 70N	700	67.000
	70CB	้ 70ท '	71N	70.330
10	70CB	70N	70CG	10.490
	70C	70N	700	24.900
	70C	70N	71N	17.080
	70C	70N	70CG	55.470
	700	70N	71N	40.450
15	700	70N	70CG	64.880
	71N	70N	70CG	61.620
	70N	70CA	70CB	106.91
	70N	70CA	70C	110.27
	70N	70CA	700	94.920
20	70N	70CA	71N	123.39
	70N	70CA	70CG	137.63
	70N	70CA	70CD1	150.73
	70n	70CA	70CD2	130.99
	70N	70CA	71CA	120.25
25	, 70CB	70CA	. 70C	109.97
	70CB	70CA	700	95.430
	70CB	70CA	. 71N	121.60
	70CB	70CA	70CG	31.050
	70CB	70CA	70CD1	54.880
30	70CB	70CA	70CD2	25.460
	70CB	70CA	71CA	118.53
	70C	70CA	700	26.590
	70C	70CA	71N	29.160
	70C	70CA	70CG	96.100
35	70C	70CA	70CD1	98.220
	70C	70CA	70CD2	90.820
	70C	70CA	71CA	20.220
	700	70CA	71N	55.750
	700	70CA	70CG	94.790
40	700	70CA	70CD1	108.55
	. 700	70CA	70CD2	84.990
	700	70CA	71CA	46.810
	71N	70CA	70CG	95.770
				473

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	71N	70CA	70CD1	85.040
	71N	70CA	7,0CD2	96.710
	71N	70CA	71CA	8.940
	70CG	7.0CA	70CD1	26.790
5	70CG	70CA	70CD2	12.590
	70CG	70CA	71CA	95.830
	70CD1	70CA	70CD2	38.940
	70CD1	· 70CA	71CA	88.910
	70CD2	70CA	71CA	94.810
10	70CG	70CB	70CA	117.56
	70CG	70CB .	70N	152.70
	70CG	70CB	. 70C	100.55
٠.	. 70CG	70CB	70CD2	28.640
	70CG	70CB	70CD1	28.170
15	70CG	70CB	700	106.07
	70CG	70CB	71N	87.340
	70CG	.70CB	70CE2	19.310
	70CG	70CB	70CE1	18.640
	70CA	70CB	70N	35.640
20	70CA	70CB	70C	35.040
	70CA	70CB	70CD2	139.47
	70CA	70CB	70CD1	95.650
	70CA	70CB · · ·	700 .	53,800
	70CA	70CB	71N	36.510
25	70CA	70CB	70CE2	134.74
	70CA	70CB	70CE1	105.29
	70N	70CB	70C	60.030
	70N	70CB	70CD2	168.48
	70N .	70CB	70CD1	127.04
30	70N	70CB	700	64.910
	70N	70CB	71N	69.250
	70N	70CB	70CE2	170.05
	70N	70CB	70CE1	137.27
	70C	70CB	70CD2	110.54
35	70C	70CB	70CD1	92.340
	70C	70CB	700	24.450
	70C	70CB	71N	17.380
	70C	70CB .	70CE2	110.50
	70C	70CB	70CE1	98.260
40	70CD2	70CB	70CD1	56.640
	70CD2	70CB	700	103.72
	70CD2	70CB	71N	103.59
	70CD2	70CB	70CE2	10.040
	•		•	474

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	70CD2	70CB	70CE1	46.680
	70CD1	70CB	700	108.56
	70CD1	70CB	71N	75.480
	70CD1	70CB	70CE2	46.880
5	70CD1	70CB	70CE1	10.230
	7,00	70CB	71N	40.070
	700	70CB	70CE2	107.98
	700	70CB	70CE1	111.25
	71N	70CB	70CE2	100.81
10	71N	70CB	70CE1	82.170
•	70CE2	70CB	70CE1	36.820
	70CD1	70CG	70CD2	118.06
	70CD1	70CG	70CB	121.18
	70CD1	70CG	70CE2	88.760
15	70CD1	70CG	70CE1	29.500
	70CD1	70CG	70CA	96.460
	70CD1	70CG	70CZ	59.020
	70CD1	70CG	70C	98.630
	70CD1	70CG	700	115.86
20	70CD1	70CG	71N	80.340
	70CD1	70CG	70N	106.78
	70CD2	70CG	70CB	120.20
	70CD2	70CG	70CE2	29.310
	70CD2	70CG	70CE1	88.570
25	70CD2	70CG	70CA	143.55
	70CD2	70CG	70CZ	59.050
	70CD2	70CG	70C	125.91
	70CD2	70CG	700	108.07
	70CD2	70CG	71N	130.21
30	70CD2	70CG	70N	135.15
	70CB	70CG	70CE2	148.81
	70CB	70CG	70CE1	149.97
	70CB	70CG	70CA	31.380
	70CB	. 70CG	70CZ	171.65
35	70CB	70CG	70C	51.310
	70CB	70CG	700	50.730
	70CB	70CG	71N	68.810
	70CB	70CG	70N	16.810
	70CE2	70CG	70CE1	59.270
40	70CE2	70CG	70CA	167.45
	70CE2	70CG	70CZ	
	70CE2	70CG		
	70CE2	70CG	700	126.97
				475

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	70CE2	70CG	71N	130.33
	70CE2	70CG	, 70N	164.45
	70CE1	70CG	70CA	125.33
	70CE1	70CG	70CZ	29.530
5	70CE1	70CG	70C	120.26
	70CE1	70CG .	700	132.40
	70CE1	70CG	71N	100.25
	70CE1	70CG	70N	136.28
	70CA	70CG	70CZ	153.44
10	70CA	70CG	70C	28.840
	70CA	70CG	700	40.600
	70CA	70CG	71N	40.450
	70CA	70CG	70N	15.000
	70CZ	70CG	70C	136.67
15	70CZ	70CG	700	137.52
	70CZ	70CG	71N	118.53
	70CZ	.70CG	70N	165.80
	70C	70CG	700	18.990
	70C	70CG	71N	20.040
20	70C	70CG	70N	39.910
	. 700	70CG	71N	35.520
	700	70CG	70N	45.860
	71N	70CG∴	70N	54.640
	70CG	70CD1	70CE1	121.21
25	70CG	70CD1	70CD2	30,980
	70CG	70CD1	70CZ	91.090
	70CG	70CD1	70CB	30.650
	70CG	70CD1	70CE2	60.970
	70CG	70CD1	70CA	56.760
30	70CG	70CD1	70C	58.990
	70CG	70CD1	700H	101.71
	70CG	70CD1	71N	78.140
	70CE1	70CD1	70CD2	90.240
	70CE1	70CD1	70CZ	30.130
35	70CE1	70CD1	70CB	151.11
	70CE1	70CD1	70CE2	60.240
	70CE1	70CD1	70CA	170.56
	70CE1	70CD1	70C	146.02
	70CE1	70CD1	700H	19.540
40	70CE1	70CD1	71N	131.69
	70CD2	70CD1	70CZ	60.120
	70CD2	70CD1	70CB	61.440
	70CD2	70CD1	70CE2	30.000
				176

	70CD2	70CD1	70CA	87.180
	70CD2	70CD1	70C	83.720
	70CD2	70CD1	700H	70.760
•	70CD2	70CD1	71N	98.740
5	70CZ	70CD1	70CB	121.24
	70CZ	70CD1	70CE2	30.120
	70CZ	70CD1	70CA	146.25
	70CZ	70CD1	70C	131.84
	70CZ	70CD1	700H	10.700
10	70CZ	70CD1	71N	131.06
•	70CB	70CD1	70CE2	91.290
	70CB	70CD1	70CA	29.480
	70CB	70CD1	70C	43.450
	70CB	70CD1	700H	131.64
15	70CB	70CD1	71N	63.770
	70CE2	70CD1	70CA	116.79
	70CE2	70CD1	70C	108.68
	70CE2	70CD1	700H	40.770
	70CE2	70CD1	71N	117.73
20	70CA	70CD1	70C	24.590
	70CA	70CD1	700H	156.75
	70CA	70CD1	71N	40.160
	70C	70CD1	700H	139.51
1	70C	70CD1	71N	20.610
25 ,	70OH	70CD1	71N	134.22
	70CZ	70CE1	70CD1	119.14
	70CZ	70CE1	700H	30.030
	70CZ	70CE1	70CE2	29.880
	70CZ	70CE1	70CG	89.850
30	70CZ	70CE1	70CD2	59.730
	70CZ	70CE1	70CB	100.75
	70CD1	70CE1	700H	149.06
	70CD1	70CE1	70CE2	89.270
	70CD1	70CE1	70CG	29.290
35	70CD1	70CE1	70CD2	59.420
	70CD1	70CE1	70CB	18.660
	70OH	70CE1	70CE2	59.890
	70ОН	70CE1	70CG	119.81
	70OH	70CE1	70CD2	89.720
40	70OH	70CE1	70CB	130.48
	70CE2	70CE1	70CG	59.990
	70CE2	70CE1	70CD2	29.850
	70CE2	70CE1	70CB	70.960
				177

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	70CG	70CE1	70CD2	30.130
	70CG	70CE1	70CB	11.390
	70CD2	70CE1	70CB	41.200
	70CE2	70CD2	70CG	121.11
5	70CE2	70CD2	70CD1	90.150
	70CE2	70CD2	70CZ	30.070
	70CE2	70CD2	70CB	151.47
	70CE2	70CD2	70CE1	59.810
	70CE2	70CD2	700H	19.220
10	70CE2	70CD2	70CA	143.09
	70CG	70CD2	70CD1	30.960
	70CG	70CD2	70CZ	91.040
	70CG	70CD2	70CB	31.150
	70CG	70CD2	70CE1	61.300
15	. 70CG	70CD2	700H	101.91
	70CG	70CD2	70CA	23.850
•	70CD1	70CD2	70CZ	60.090
	70CD1	70CD2	70CB	61.930
	70CD1	70CD2	70CE1	30.340
20	70CD1	70CD2	700H	70.980
	70CD1	70CD2	70CA	53.880
	70CZ	70CD2	70CB	121.70
,	70CZ	70CD2	70CE1	29.750
	70CZ	70CD2	700H	10.950
25	. 70CZ	70CD2	70CA	113.46
	70CB	70CD2	70CE1	92.130
	70CB	70CD2	, 700Н	132.34
	70CB	70CD2	70CA	15.060
	70CE1	70CD2	700H	40.660
30	70CE1	70CD2	70CA	83.920
	700н	70CD2	70CA	124.41
	70CD2	70CE2	70CZ	119.98
	70CD2	70CE2	700H	149.77
,	70CD2	70CE2	70CE1	90.330
35	70CD2	70CE2	70CG	29.590
	70CD2	70CE2	70CD1	59.850
	70CD2	70CE2	70CB	18.490
	70CZ	70CE2	700H	29.900
	70CZ	70CE2	70CE1	29.650
40	70CZ	70CE2	70CG	90.400
	.70CZ	70CE2	70CD1	60.140
	70CZ	70CE2	70CB	101.79
	700Н	70CE2	70CE1	59.530
				478

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	700H	.70CE2	70CG	120.21
	700H	70CE2	70CD1	89.990
	700H	70CE2	70CB	131.38
	70CE1	70CE2.	70CG	60.750
5	70CE1	70CE2	70CD1	30.480
	70CE1	70CE2	70CB	72.220
	70CG	70CE2	70CD1	30.260
	70CG	70CE2	70CB	11.880
	70CD1	70CE2	70CB	41.820
10	700H	70CZ	70CE1	119.71
	700Н	70CZ	70CE2	119.76
	700H	70CZ	70CD1	150.31
	700H	70CZ	70CD2	149.60
	700H	70CZ	70CG	176.52
15	70CE1	70CZ	70CE2	120.47
	70CE1	70CZ	70CD1	30.730
	70CE1	70CZ	70CD2	90.520
	70CE1	70CZ	70CG	60.620
	70CE2	70CZ	70CD1	89.750
20	70CE2	70CZ	70CD2	29.950
	70CE2	70CZ	70CG	59.860
	70CD1	70CZ	70CD2	59.800
	70CD1	70CZ	70CG	29.890
	70CD2	70CZ	70CG	29.910
25	70CZ	700н	70CE1	30.260
	70CZ	700Н	70CE2	30.340
	70CZ	70OH	70CD2	19.450
	70CZ	700Н	70CD1	18.980
	70CE1	700Н	70CE2	60.580
30	70CE1	700H	70CD2	49.620
	70CE1	700н	70CD1	11.390
	70CE2	700н	70CD2	11.010
	70CE2	700н	70CD1	49.240
	70CD2	700н	70CD1	38.260
35	700	70C	71N	123.14
	700	70C	70CA	120.09
	700	70C	71CA	92.570
	700	70C	70N	99.070
	700	70C	70CB	99.330
40	700	70C	71C	78.860
	. 700	70C	70CG	105.60
	700	70C	72N	56.760
	700	70C	70CD1	125.74
				479

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	700		70C	71CB	108.48
	700		70C	, 710	90.870
	700		70C	27CE	75.140
	71N	'	.70C	70CA	116.77
5	71N	•	70C	71CA	30.570
	71N		70C	70N	130.09
	71N		70C	70CB	128.41
•	71N	•	70C	, 71C	50.660
	71N		70C	70CG	105.64
10	71N		70C	72N	71.070
	71N		70C	70CD1	85.130
	71N		70C	71CB	15,220
	71N		70C	710	47.160
	71N		70C	27CE	81.520
15	70CA		70C	71CA	147.33
	70CA		70C	70N	33.980
	70CA		70C	70CB	34.980
	70CA		70C	71C	149.00
	70CA		70C	70CG	55.070
20	70CA		70C	72N	156.37
	70CA	,	70C	70CD1	57.190
	70CA		70C	71CB	131.27
	70CA	••	70C:		132.91:
	70CA		70C	27CE	115.72
25	71CA	·	70C	70N	149.80
	71CA		70C	70CB	147.07
	71CA		70C	71C	29.080
	71CA		70C	70CG	118.97
	71CA		70C	72N	43.930
30	71CA	·	70C	70CD1	104.65
	71CA		70C	71CB	16.560
	71CA		70C	710	36.650
	71CA		70C	27CE	70.660
	70N		70C	70CB	57.950
35	70N		70C	71C	177.02
	70N		70C	70CG	84.620
	70N		70C	72N	155.82
	70N		70C	70CD1	90.970
	70N		70C	71CB	137.64
40	70N		70C	710	166.83
	70N		70C	27CE	85.480
	70CB		70C	71C	124.36
	70CB		70C	70CG	28.140
	*				480

	70CB	70C	72N	121.93
	70CB	70C	70CD1	44.210
	70CB	70C	71CB	142.05
	70CB	. 70C	710	112.09
5	70CB	70C	27CE	142.09
	71C	70C	70CG	97.990
	71C	70C	72N	22.120
	71C	70C	70CD1	91.980
	71C	70C	71CB	42.180
10	71C	70C	710	16.150
•	71C	70C	27CE	91.900
	70CG	70C	72N	101.82
	70CG	70C	70CD1	22.380
	70CG	70C	71CB	116.61
15	70CG	70C	710	84.400
	70CG	70C	27CE	170.06
4	72N	70C	70CD1	103.85
	72N	70C	71CB	59.890
	72N	70C	· 710	35.310
20	72N	70C	27CE	86.930
	70CD1	70C	71CB	97.910
	70CD1	70C	710	76.150
	70CD1 .	70C	27CE	159.11
	71CB	70C	710	44.150
25	71CB	70C	27CE	71.800
	710	70C	27CE	105.54
	70C	700	71N	29.440
	70C	700	70CA	33.310
	70C	700	71CA	61.030
30	70C	700	70N	56.030
	70C	700	70CB	56.220
	70C	700	72N	103.35
	70C	700	71C	78.330
	70C	700	27N	162.85
35	70C	700	70CG	55.410
	70C	700	27CE	86.530
	70C	700	27CB	134.75
	70C	700	27CA	157.10
	71N	700	70CA	62.750
40	71N	700	71CA	31.590
	71N	700	70N	82.720
	71N	700	70CB	82.340
•	71N	700	72N	77.000
				481

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	W	O 03/048733				PCT/US02/38715				
		71N	700	71C	52.450					
		71N	700	27N	157.23					
		71N	700	70CG	73.420					
		71N	700	27CE	76.870					
	. 5	71N	700	27CB	118.58					
		71N	700	27CA	137.77					
		70CA	700	71CA	94.340	·				
		70CA	700	70N	29.900					
		70CA	700	70CB	30.770					
	10	70CA	700	72N	131.80					
		70CA	700	71C	108.22					
		70CA	700	27N	134.37					
		70CA	700	70CG	44.610					
		70CA	700	27CE	98.600					
*	15	70CA	700	27CB	137.96					
		70CA	700	27CA	147.24					
		71CA	700	70N	111.73					
		71CA	700	70CB	110.81					
,		71CA	700	72N	49.690					
	20	71CA	700	71C	29.600					
		71CA	700	27N	128.54					
m.		71CA	700	70CG	95.550					
	•	71CA	700	27CE	, 70.170					
	25	71CA	700	27CB	95.820	1				
	25	71CA	700	27CA	109.66	2				
		70N	700	70CB	48.090					
		70N	700	72N	159.36					
		70N	700	71C	134.32					
	20	70N	700	27N	108.05					
	30	70N	700	70CG	69.260					
		70N	700	27CE	82.110					
		70N	700	27CB	109.82	·				
•		70N	700 700	27CA	117.61 124.02					
	35	70CB 70CB	700	72N 71C	109.62					
	. J.J	70CB	700	27N	119.93					
		70CB	700	70CG	23.200					
		70CB	700	70CG 27CE	128.06					
		70CB	700	27CB	149.98					
	40	70CB	700	27CB	139.34	•				
	-10	72N	700	71C	25.040					
		72N	700	27N	92.310					
		72N	700	70CG	100.85					
•		. 21.	, 55							
					482	•				
						•				
	•					*				

	72N	700	27CE	96.810
	72N	700	27CB	83.640
	72N	700	27CA	80.850
	· 71C	700	27N	116.95
5	71C	700	70CG	87.670
	71C	700	. 27CE	94.180
	71C	700	27CB	100.37
	71C	. 700	27CA	103.44
	27N	700	70CG	128.88
10	27N	700	27CE	84.660
	27N	700	27CB	39.280
	27N	700	27CA	19.550
	70CG	700	27CE	140.73
	70CG	700	27CB	167.97
15	70CG	700	27CA	146.72
	27CE	700	. 27CB	48.260
	27CE	700	27CA	70.590
	27CB	700	27CA	22.440
	70C	71N	71CA	122.07
20	70C	71N	700	27.430
	70C	71N	70CA	34.070
	70C	71N	71CB	156.58
	70C	· 71N	71C	105.29
	70C	71N	710	114.85
25	70C	71N	72N	87.060
	70C	71N	70N	32.830
	70C	71N	, 70CB	34.210
	70C	71N	70CG	54.320
	70C	71N	70CD1	74.260
30	70C	71N	27CE	79.190
	71CA	71N	700	94.650
	71CA	71N	70CA	156.14
	71CA	71N	71CB	35.960
	71CA	71N	71C	34.730
35	71CA	71N	710	47.910
	71CA	, 71N	72N	41.570
	71CA	71N	70N	144.29
	71CA	71N	70CB	143.42
	71CA	71N	70CG	
40	71CA	71N	70CD1	131.98
	71CA	71N	27CE	76.210
	700	71N	70CA	61.500
	700	71N	71CB	129.74
				483

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		700	71N	71C	82.170	. ,
,	•	700	71N	710	97.500	•
		700	71N	72N	62.170	•
		700	· 71N	70N	56.830	
	5	700	71N	70CB	57.590°	
	•	700	71N	70CG	71.060	
		700	71N	70CD1	92.580	* .
		700	71N	27CE	69.480	
		70CA	71N	71CB	166.85	
	10	70CA	71N	71C	131.75	
		70CA	71N	710	129.72	•
		70CA	71N	72N	117.88	
		70CA	71N	70N	20.640	
		70CA	71N	70CB	21.890	
	15	70CA	71N	70CG	43.780	•
		70CA	71N	70CD1	54.810	
		70CA	71N	27CE	94.230	
		71CB	71N	71C	60.910	•
		71CB	71N	710	59.960	
	20	71CB	71N	72N	75.260	
		71CB	71N	70N	153.78	·
		71CB	71N	70CB	164.62	
		71CB	71N	. 70CG.	1.40.81	
		71CB	71N	70CD1	124.74	•
•	25	71CB	71N	27CE	85.200	
		71C	71N	710	21.860	
		71C	71N	72N	20.690	·
		71C	71N	70N	138.03	•
		71C	71N	70CB	111.76	
	30	71C	71N	70CG	96.900	·
		71C	71N	70CD1	100.26	
		71C	71N	27CE	101.90	
		710	71N	72N	40.850	
		710	71N	70N	145.40	
	35	710	71N	70CB	107.84	
		710	71N	70CG	87.250	
		710	71N	70CD1	84.080	
		710	71N	27CE	122.09	
		72N	71N	70N	118.89	
	40	72N	71N	70CB	101.86	
		72N	71N	70CG	94.280	
		72N	71N	70CD1	104.97	
		72N	71N	27CE	89.110	
	• •				484	4

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W O 05/040/55	1 C1/0502/00/15

			70N	71N	70CB	40.420						
			70N	71N	70CG	63.740		• '				
			70N	71N	70CD1	75.300			•			
			70N	71N	27CE	73.750				,		
•	5		70CB	71N	70CG	23.840			F			
•		+	70CB	71N '	. 70CD1	40.740	•	•				
			70CB	71N	27CE	109.99	•					
•			70CG	. 71N	70CD1	21.520						
			70CG	71N	27CE	133.04						
	10		70CD1	71N	27CE	149.03	·			•		
			71N	71CA	71CB	109.56	•	•				
			71N	71CA	71C	112.75		•				
			71N	71CA	710	105.38						
			71N	71CA	70C	27.360						
	15		71N	71CA	72N	115.21						,
			71N	71CA	700	53.760						
			.71N	71CA	70CA	14.920	•					
			71N	·71CA	72CA	115.46					1	
			· 71N	71CA	27CE	82.300						
	20		71CB	71CA	71C	109.60	1					
			71CB	71CA	710	89.910						
			71CB	71CA	70C	136.21						
			71CB	71CA	72N	128.74	Salmana a recordo	,				,
			71CB	71CA	700	160.54						
	25		71CB	71CA	70CA	124.20			. •			
			71CB	71CA	72CA	123.62						
			71CB	71CA	. 27CE	102.93						
			71C	71CA	710	26.360	•					
			71C	71CA	70C	101.06						
	30		71C	71CA	72N	29.260						
			71C	71CA	700	87.880						
			71C	71CA	70CA	106.58	٠.					
			71C	71CA	72CA	20.910		•		•		
	0.5		71C	71CA	27CE	135.72	•					·
	35		710	71CA	70C	106.32						8
			710	71CA	72N	55.620	•					
			710	71CA	700	103.70	•					
			710	71CA	70CA	106.14						
	40		710	71CA	72CA	47.270						
	40		710	71CA	27CE	162.06						
			70C	71CA	72N	92.660						
			7,0C	71CA	700 700	26.400						
			70C	71CA	70CA	12.450						
					•	485						

	70C	71CA	72CA	95.460	
	70C	71CA	.27CE	72.980	
	72N	71CA	700	70.710	
	72N	71CA	70CA	102.91	
5	72N	71CA	72CA	8.350	
	72N	71CA ·	27CE	106.47	
	700	71CA	70CA	38.850	
•	700	71CA	72CA	75.600	
	700	71CA	27CE	67.380	
10	70CA	71CA	72CA	104.61	
	70CA	71CA	27CE	77.110	
	72CA	71CA	27CE	114.81	•
	71CA	71CB	. 71N	34.470	
	71CA	71CB	71C	35.620	•
15	71CA	71CB	710	57.930	
	71CA	71CB	72N	32.120	
	71CA	71CB	70C	27.230	•
	71N	71CB	71C	61.000	· ·
	71N	71CB	710	72.360	
20	71N	71CB	72N	64.020	
	71N	71CB	70C	8.190	
	71C	71CB	710	25.670	4
	· 71C	71CB	. · ·72N · ·		Calman and the second of the s
	71C	71CB	70C	56.950	
25	710	71CB	72N	39.060	
	710	71CB	70C	71.620	
	72N	71CB	70C	58.090	
	710	71C	72N	123.77	
	710	71C	71CA	119.82	
30	710	71C	72CA	93.990	
	710	71C	71CB	92.930	•
	710	71C	71N	109.08	
	710	71C	70C	119.12	
25	710	71C	700	134.27	
35	710	71C	72CB	88.520	•
	72N	71C	71CA	116.41	
	72N	71C	72CA	29.780 137.30	•
	72N	71C	71CB		
40	72N	71C	71N 70C	118.01 96.550	
40	72N	71C	700	73.760	
	72N	71C	700 72CB	43.410	
	フつい				
	72N	71C			
	72N 71CA	71C	72CA	146.18 486	•

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	71CA	71C	71CB	34.780
	71CA	71C	71N	32.530
	71CA	71C	70C	49.860
	71CA	71C	700	62.520
5	71CA	71C	72CB	141.88
	72CA	71C	71CB	155.41
	72CA	71C	71N	139.72
	72CA	71C	70C	115.69
	72CA	71C	700	94.990
.10	72CA	71C	72CB	27.030
	71CB	71C	71N	58.090
	71CB	71C	70C	80.870
	71CB	71C	700	96.960
	71CB	71C	72CB	129.92
15	71N	71C	70C :	24.050
	71N	71C	700	45.370
	71N	71C	72CB	161.09
	70C	71C	700	22.810
	70C	71C	72CB	139.51
20	700	71C	72CB	116.94
	71C	710	72N	29.380
	71C	710	71CA	33.810
	71C	710	72CA	60.310
	71C ·	710	71CB	61.410
25.	71C	710	71N	49.060
	71C	710	72CB	70.480
	71C	710	70C	44.730
	72N	710	71CA	63.190
	72N	710	72CA	30.930
30	72N	710	71CB	88.790
	72N	710	71N	74.700
	72N	710	72CB	45.310
	72N	710	70C	64.140
	71CA	710	72CA	94.120
35	71CA	710	71CB	32.160
	71CA	710	71N	26.700
	71CA	710	72CB	100.98
	71CA	710	70C	37.030
	72CA	710	71CB	117.50
40	72CA	710	71N	102.84
	72CA	710	72CB	26.060
	72CA	710	70C	88.620
	71CB	710	71N	47.680
				107

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	71CB	710	72CB	111.77
	71CB	710	70C	64.230
	71N	710	72CB	119.19
	71N	710	70C	17.990
5	72CB	710	70C	109.31
	71C	72N	72CA	123.26
	. 71C	72N	710	26.850
	71C	72N	72CB	114.53
	71C	72N	71CA	34.330
10	71C	72N	700	81.190
	71C	72N	270	146.86
	71C	72N	71N	41.300
	71C	72N	70C	61.330
	71C	72N	71CB	28.090
15	· 71C ·	72N	72CG	120.73
	72CA	72N	710	96.410
	72CA	72N	72CB	36.130
	72CA	72N	71CA	157.59
	72CA	72N	700	130.94
20	72CA	72N	270	87.240
	72CA	72N	71N	149.24
	72CA	72N	70C	139.50
•	72CA	72N	·71CB ·	143.24
	72CA	72N	72CG	24.380
25	710	72N	72CB	93.520
	710	72N	71CA	61.190
	710	72N	700	99.610
	710	72N	270	166.12
	710	72N	71N	64.450
30	710	72N	70C	80.560
	710	72N	71CB	52.140
	710	72N	72CG	96.790
	72CB	72N	71CA	136.83
	72CB	72N	700	163.29
35	72CB	72N	270	81.510
	72CB	72N	71N	155.58
	72CB	72N	70C	172.50
	72CB	72N	71CB	117.74
	72CB	72N	72CG	12.020
40	71CA	72N	700	59.600
	71CA	72N	270	114.35
	71CA	72N	71N	23.230
	71CA	72N	70C	43.410
				488

	71CA	72N	71CB	19.140
	71CA	72N,	72CG	147.56
	700	72N	270	87.890
	700	72N	71N ·	40.840
5	700	72N	70C	19.890
	700	72N	· 71CB	78.740
	700	72N	72CG	152.63
	270	72N	71N	117.30
	270	. 72N	. 70C	105.29
10	270	72N	71CB	119.05
	270	72N	72CG	81.040
	71N	72N	70C	21.880
	71N	72N	71CB	40.720
	71N	72N	72CG	161.22
15	70C	72N	71CB	62.020
	70C	72N	72CG	163.70
	71CB	, 72N	72CG	128.46
	72N	72CA	72CB	109.52
	72N	72CA	· 71C	26.960
20	72N	72CA	72CG	141.87
	72N	72CA	710	52.660
	72N	72CA	72CD2	146.65
	72N'	72CA	72CD1	139.86
	72N	72CA	270	68.520
25	. 72N	72CA	71CA	14.060
	72CB	· 72CA	71C	105.89
	72CB	72CA	72CG	32.600
	72CB	72CA	710	99.550
	72CB	72CA	72CD2	44.050
30	72CB	72CA	72CD1	43.570
	72CB	72CA	270	87.730
	72CB	72CA	71CA	107.84
	71C	72CA	72CG	135.26
	71C	72CA	710	25.700
35	71C	72CA	72CD2	126.95
	71C	72CA	72CD1	148.66
	71C	72CA	270	94.770
	71C	72CA	71CA	12.900
	72CG	72CA	710	119.79
40	72CG	72CA	72CD2	21.870
	72CG	72CA		21.560
	72CG	72CA	270	97.590
	72CG	72CA	71CA	139.89
	•			489

	•	710	72CA	72CD2	104.93		•	
		710	72CA	72CD1	140.32	•		
		710	72CA	270	119.83		•	•
		710	7.2CA	71CA	38.610			•
	5	72CD2	72CA	72CD1	41.260		· ·	
		72CD2	72CA	270	119.45			
		72CD2 ·	72CA	71CA	136.99			
		72CD1	72CA ,	270	79.620			
		72CD1	72CA	71CA	146.25			
	10	270	72CA	71CA	82.130		•	•
		72CG	72CB	72CA	114.08			
		72CG	72CB	. 72N	148.14	•		
		72CG	72CB .	72CD2	28.400			
		72CG	72CB .	72CD1	28.260		1	
	15	72CG	72ÇB	71C	153.74		•	1
		72CG .	72CB	710	137.43			
		72CG	.72CB	72CE2	18.460	•		,
		72CG	72CB	72CE1	18.190			
	•	72CG	72CB .	270	114.19		•	
	20	72CA	72CB -	72N	34.350			
		72CA .	72CB	72CD2	110.80	•		
		72CA	72CB	72CD1	111.57			
		72CA	72CB	71C	47.080	Catholic Committee Committ		
		72CA	72CB	710	54.380	•		
•	25	72CA	72CB	72CE2	112.85			1
		72CA	72CB	72CE1	113.46			
		72CA	72CB	270	68.670			•
		72N	72CB	72CD2	140.56	•		
		72N	72CB	72CD1	136.51			
	30	72N	72CB	71C	22.060			•
		72N	72CB	710	41.170			
		72N	72CB	72CE2	145.55	٠,		
		72N	72CB	72CE1	142.65			
		72N	72CB	270	59.200			
	35	72CD2	72CB	72CD1	56.660			
		72CD2	72CB	71C	130.98			
		72CD2	72CB	710	111.11		•	
		72CD2	72CB	72CE2	9.950		•	
		72CD2	72CB	72CE1	46.590			·
	40	72CD2	72CB	270	141.36			
		72CD1	72CB	71C	157.53			
		72CD1	72CB	710	159.45			
		72CD1	72CB	72CE2	46.710			
					490			

	72CD1	72CB	72CE1	10.080
	72CD1	72CB	270	86.740
	71C	72CB	710	20.990
	71C	-72CB	72CE2	139.78
5	71C	72CB	72CE1	160.44
	71C	72CB	270	78.680
	710	72CB	72CE2	120.56
	710	72CB	72CE1	152.99
	710	72CB	270	99.520
10	72CE2	72CB	72CE1	36.640
•	72CE2	72CB	270	132.04
	72CE1	72CB	270	96.610
	72CD2	72CG	72CD1	118.70
	72CD2	72CG	72CB	120.48
15	72CD2	72CG	72CE2	29.700
	72CD2	72CG	72CE1	88.910
	72CD2	72CG	72CA	114.81
	72CD2	72CG	72CZ	59.270
	72CD2	72CG	72N	120.43
20	72CD1	72CG	72CB	120.81
	72CD1	72CG	72CE2	89.010
	72CD1	72CG	72CE1	29.800
	72CD1	72CG	72CA	115.91
•	72CD1	72CG	72CZ	59.430
25 ,	72CD1	72CG	72N	117.10
	72CB	72CG	72CE2	150.17
	72CB	72CG	72CE1	150.61
	72CB	72CG	72CA	33.320
	72CB	72CG	72CZ	179.28
30	72CB	72CG	72N	19.840
	72CE2	72CG	72CE1	59.210
	72CE2	72CG	72CA	136.56
	72CE2	72CG	72CZ	29.580
	72CE2	72CG	72N	146.64
35	72CE1	72CG	72CA	137.55
	72CE1	72CG	72CZ	29.630
	72CE1	72CG	72N	143.84
	72CA	72CG	72CZ	147.36
	72CA	72CG	72N	13.750
40	72CZ	72CG	72N	160.86
	72CG	72CD1	72CE1	120.63
	72CG	72CD1	72CD2	30.630
	72CG	72CD1	72CZ	90.830
				491

	72CG	72CD1	72CB	30.930
	72CG	72CD1	72CE2	60.910
	72CG	72CD1	280D1	142.39
	72CG	72CD1	28CG	124.62
5	72CG	72CD1	72CA	42.530
	72CG	72CD1 ·	280D2	106.03
	72CG	72CD1	28CA	122.27
	72CE1	72CD1	72CD2	90.000
	72CE1	72CD1	72CZ	29.800
10	72CE1	72CD1	72CB	151.55
	72CE1	72CD1	72CE2	59.720
	72CE1	72CD1	280D1	61:780
	72CE1	72CD1	28CG	80.270
	72CE1	72CD1,	72CA	147.38
15	72CE1	72CD1	280D2	83.110
	72CE1	72CD1	28CA	110.27
	72CD2	72CD1	72CZ	60.200
	72CD2	72CD1	72CB	61.560
	72CD2	72CD1	72CE2	30.280
20	72CD2	72CD1	280D1	129.67
	72CD2	72CD1	28CG	123.86
	72CD2	72CD1	72CA	68.940
	· 72CD2 ··	72CD1	280D2	104.25
	72CD2	72CD1	28CA	145.48
25	72CZ	72CD1	72CB	121.76
	72CZ	72CD1	72CE2	29.920
	72CZ	72CD1	280D1	84.600
	72CZ	72CD1	28CG	97.410
	72CZ	72CD1	72CA	123.48
30	72CZ	72CD1	.280D2	90.960
	72CZ	72CD1	28CA	135.19
	72CB	72CD1	72CE2	91.840
	72CB	72CD1	280D1	136.58
	72CB	72CD1	·28CG	115.00
35	72CB	72CD1	72CA	24.860
	72CB -	72CD1	280D2	103.47
	72CB	72CD1	28CA	95.310
	72CE2	72CD1	280D1	108.17
	72CE2	72CD1	28CG	113.24
40	72CE2	72CD1	72CA	96.530
	72CE2	72CD1	280D2	98.660
	72CE2	72CD1	28CA	152.31
	280D1	72CD1	28CG	21.660
	•			492

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	280D1	72CD1	72CA	112.55
	280D1	72CD1	280D2	37.060
	280D1	72CD1	28CA	50.620
	28CG	72CD1	72CA .	90.900
5	28CG	72CD1	280D2	20.050
	28CG	72CD1	28CA	40.080
	72CA	72CD1	280D2	78.630
	72CA	72CD1	28CA	79.860
	28OD2	72CD1	28CA	53.660
10	72CG	72CD2	72CE2	120.82
	72CG	72CD2	72CD1	30.660
	72CG	72CD2	72CZ	91.020
	72CG	72CD2	72CB	31.120
	72CG	72CD2	72CE1	61.010
15	. 72CG	72CD2	72CA :	43.310
	72CE2	72CD2	72CD1	90.160
•	72CE2	72CD2	72CZ	29.800
	72CE2	72CD2	72CB	151.94
	72CE2	72CD2	72CE1	59.810
20	72CE2	72CD2	72CA	147.84
	72CD1	72CD2	72CZ	60.360
	72CD1	72CD2	72CB	61.780
	72CD1	72CD2	72CE1	30.350
	72CD1	72CD2	72CA	69.800
25	72CZ	72CD2	72CB	122.14
	72CZ	72CD2	72CE1	30.010
	72CZ	72CD2	72CA	124.38
,	72CB	72CD2	72CE1	92.130
	72CB	72CD2	72CA	25.150
30	72CE1	72CD2	72CA	97.470
	72CZ	72CE1 ·	72CD1	120.06
	72CZ	72CE1	72CE2	30.110
	72CZ	72CE1	72CG	90.490
24	72CZ	72CE1	280D1	128.03
35	72CZ	72CE1	72CD2	60.410
•	72CZ	72CE1	28CG	126.46
	72CZ	72CE1	28OD2	109.52
	72CZ	72CE1	72CB	101.69
40	72CD1	72CE1	72CE2	89.950
40	72CD1	72CE1	72CG	29.570
	72CD1	72CE1	280D1	91.000
•	72CD1	72CE1	72CD2	59.650
	72CD1	72CE1	28CG	75.900
				403

		72CD1	72CE1	28OD2	75.000
		72CD1	72CE1	72CB	18.370
		72CE2	72CE1	72CG	60.390
		72CE2	72CE1	280D1	136,.30
5		72CE2	72CE1	72CD2	30.310
		72CE2	72CE1	28CG	123.13
		72CE2	72CE1	280D2	103.74
		72CE2	72CE1	72CB	71.590
		72CG	72CE1	280D1	111.96
10		72CG	72CE1	72CD2	30.080
		72CG	72CE1	28CG	93.450
		72CG	72CE1	280D2	83.970
		72CG	72CE1	72CB	11.210
		280D1	72CE1	72CD2	129.34
15		280D1	72CE1	28CG	19.220
		280D1	· 72CE1	28OD2	35.520
		280D1	72CE1	72CB	104.46
		72CD2	72CE1	28CG	110.49
		72CD2	72CE1	280D2	94.360
20		72CD2	72CE1	72CB	41.280
		28CG	72CE1	28OD2	19.440
		28CG	72CE1	72CB	86.970
	•	280D2	72CE1	72CB	.80.590
		72CZ	72CE2	72CD2	120.05
25	•	72CZ	72CE2	72CE1	30.170
		72CZ	72CE2	72CG	90.570
		72CZ	72CE2	72CD1	60.490
		72CZ	72CE2	72CB	101.94
		72CD2	72CE2	72CE1	89.890
30		72CD2	72CE2	72CG	29.480
		72CD2	72CE2	72CD1	59.560
		72CD2	72CE2	72CB	18.120
		72CE1	72CE2	72CG	60.400
		72CE1	72CE2	72CD1	30.320
35		72CE1	72CE2	72CB	71.770
		72CG	72CE2	72CD1	30.080
		72CG	72CE2	72CB	11.370
		72CD1	72CE2	72CB	41.450
		72CE2	72CZ	72CE1	119.73
40		72CE2	72CZ	72CD2	. 30.150
		72CE2	72CZ	72CD1	89.590
		72CE2	72CZ	72CG	59.850
		72CE2	72CZ	280D1	130.21
					494

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	72CE1	72CZ	72CD2	89.580
	72CE1	72CZ	72CD1	30.140
	72CE1	72CZ	'72CG	59.870
	72CE1	72CZ	280D1	34.880
5	72CD2	72CZ	72CD1	59.440
	72CD2	72CZ	72CG	29.700
	72CD2 .	72CZ	28OD1	105.62
	72CD1	72CZ	72CG	29.740
	72CD1	72CZ	280D1	55.110
10	72CG	72CZ	280D1	80.010

Table IIIB
Interatomic angle between residues in the active site of UPPS in complex with FPP

	VVILIT I I. I			
5	ATOM1	ATOM2	EMOTA .	ANGLE, degree
	79NH1	1C1	79NH2	36.680
	300D1	1C2	45NE2	73.500
	300D1	1C2	79NH1	123.81
	45NE2	1C2,	79NH1	54.230
10	710	1C4	71C	16.510
	710	1C5 .	45CD2	138.38
	300D1	1C6	710	158.04
	49N	1C10	450	54.930
	49N	1C10	48C	22.570
15	49N	1C10	48CA	41.710
	49N	1C10	300D1	112.37
	49N	1C10	49CA	20.490
	450	1C10	48C	66.450
	450	1C10	48CA	60.290
20	450	1C10	300D1	80.140
	450	1010	49CA	66.810
	48C	1C10	48CA	24.950
	48C	1010	300D1	98.690
	48C	1C10.,	49CA	38.030
25	48CA	1C10	300D1	73.850
	48CA	1C10	. 49CA	60.970
	300D1	1C10	49CA	132.86
	143CE2	1C14	143CZ	22.460
	143CE2	1C14	143CD2	20.550
30	143CE2	1C14	91CG	154.92
	143CE2	1C14	91CA	166.15
	143CZ	1C14	143CD2	36.950
	143CZ	1C14	91CG	161.83
	143CZ	1C14	91CA	143.89
35	143CD2	1C14	91CG	134.76
	143CD2	1C14	91CA	159.08
	91CG	1C14	91CA	34.360
	49SD	1C15	94CG	72.370
	49SD	1C15	94CB	63.260
40	49SD	1C15	94CD1	62.610
	49SD	1C15	49CG	28.760
	49SD	1C15	900	60.290

	94CG	1C15	94CB	23.960
	94CG	1C15	94CD1	22.200
	94CG	1C15	49CG	80.380
•	94CG	1C15	900	71.370
5	94CB	1C15	94CD1	40.410
	94CB	1C15	49CG	81.980
	94CB	1C15	900	47.420
	94CD1	1C15	4 9CG	61.840
	94CD1	1C15	900	84.480
10	49CG	1C15	900	89.040
	79NH2	101A	45CE1	104.86
	79NH2	101A	79NH1	36.270
	79NH2	101A	31N	161.20
	45CE1	101A	79NH1	69.380
15	45CE1	101A	31N	73.460
	79NH1	101A	31N	141.07
	79NH2	102A	280D2	143.61
	29N	103A	30N	51.620
	29N	103A	31N	98.770
20	29N	103A	29C	42.330
	29N	103A	30CB	88.140
	29N	103A	29CA	21.740
F	29N	103A	30CA	72.890
•	30N	103A	31N	53.440
25	30N	103A	29C	21.050
	30N	103A	30CB	40.610
	30N	103A	29CA	39.740
	30N	103A	30CA	21.320
	31N	103A	29C	56.440
30	31N	103A	30CB	47.440
	31N	103A	29CA	78.530
	31N	103A	30CA	38.230
	29C	103A	30CB	60.250
	29C	103A	29CA	23.500
35	29C	103A	30CA	37.980
•	30CB	103A	29CA	80.270
	30CB	103A	30CA	23.300
	29CA	103A	30CA	59.960
	29N	1PB	29CA	22.630
40	29N	1PB	29C	39.230
	29N	1PB	30N	43.180
	29N	1PB	31N	87.600
	29CA	1PB	29C	22.740

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	29CA	1PB	30N	36.770
	29CA	1PB	31N	73.860
	29C	1PB	30N	19.570
	29C	1PB	31N	51.200
5	30N	1PB	31N	45.170
	280Ď2	101B	29N	84.890
	280D2	101B	28CG	16.680
	29N	101B	28CG	68.950
	29CA	103B	32N	96.470
10	29CA	103B	32CB	86.020
	29CA	103B	29C	28.020
	29CA	103B	29N	26.430
	29CA	103B	290	41.610
	29CA	103B	30N	40.840
15	· 29CA	103B	31N	86.120
	29CA	103B	32CA	93.510
•	32N	103B	32CB	45.930
	32N	103B	29C	74.560
	32N	103B	29N	119.84
20	32N	103B	290	55.800
	32N	103B	30N	80.770
	32N	103B	31N	48.860
	32N	103B	. 32CA	22.120
	32CB	103B	29C	83.310
25	32CB	103B	29N	111.02
	32CB	103B	290	65.280
	32CB	103B	30N	101.43
	32CB	103B	31N	92.340
	32CB	· 103B	32CA	23.970
30	29C	103B	29N	45.490
	29C	103B	290	20.200
	29C	103B	30N	20.670
	29C	103B	31N	58.520
	29C	103B	32CA	79.800
35	29N	103B	290	64.150
	29N	103B	30N	45.760
	29N	. 103B	31N	93.530
	29N	103B	32CA	119.86
	290	103B	30N	36.150
40	290	103B	31N	54.170
	290	103B	32CA	59.600
	30N	103B	31N	48.360
	30N	103B	32CA	92.530
				498

31N 103B 32CA 70.170

Table IIIC
Interatomic angle between residues in the active site of UPPS in complex with IPP

5	with IPP			
	ATOM1	ATOM2	EMOTA	ANGLE, degree
	280D2	1C02	270	87.520
•	280D2	1C02	28CB	36.210
	270	1C02	28CB	61.460
10	710	1C05	700	72.200
	710	1C05	71C	21.680
	710	1C05	. 72N	37.100
	710	1C05	70C	69.880
	710	1C05	72CA	46.020
15	710	1C05	76ND2	106.01
	700	1C05	71C	62.240
	700	.1C05	72N	74.850
	700	1C05	70C	17.710
	700	1C05	72CA	96.890
20	700	1C05	76ND2	166.88
	71C	1C05	72N	20.700
	71C	1C05	70C	54.260
	· · · 71C · ·	1C05	72CA	38.940
	71C	1C05	76ND2	111.29
25	72N	1C05	70C	61.890
	72N	1C05	72CA	22.050
	72N	1C05	76ND2	95.800
	70C	1C05	72CA	83.310
	70C	. 1C05	76ND2	149.20
30	72CA	1C05	76ND2	73.940
	70CD2	1C09	70CE2	21.400
	70CD2	1C09	70CG	21.670
	70CE2	1C09	70CG	37.390
	70CE2	1C12	70CD2	21.540
35	200NH2	1014	2080G	65.400
	200NH2	1014	208CB	73.390
	2080G	1014	208CB	19.950
	280D2	1P15	200NH2	73.130
	76ND2	1016	760D1	39.750
40	76ND2	1016	76CG	20.700
	76ND2	1016	250CA	101.94
	76ND2	1016	730G	42.420

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	760D1	1016	7 6CG	19.460
	760D1	1016	250CA	65.930
	760D1	1016	730G	64.870
	76CG	1016	250CA	82.090
5	76CG	1016	730G	49.850
	250CA	1016	730G	95.020
	200NH2	1017	280D2	79.710
	200NH2	1017	28CG	64.100
	280D2	1017	28CG	18.170
10	280D2	1018	28CG	16.510
	280D2	1018	247NH2	84.690
	280D2	1018	280D1	30.030
	28CG	1018	247NH2	88.990
	28CG	1018	280D1	17.610
15	247NH2	1018	280D1	77.660
	2080G	1P19	250CA	119.39
	2080G	1P19	206NH1	91.290
	2080G	1P19	2470	124.73
	2080G	1P19	206CD	51.730
20	250CA	1P19	206NH1	134.73
	250CA	1P19	2470	54.230
	250CA	1P19	206CD	138.68
	206NH1	1P19	2470	81.340
	206NH1	1P19	206CD	41.710
25	2470	1P19	206CD	95.200
	2080G	1020	250N	151.34
	2080G	1020	250CA	158.25
	2080G	1020	217CE2	77.450
	2080G	1020	208CB	22.490
30	2080G	1020	2470	144.34
	250N	1020	250CA	25.390
	250N	1020	217CE2	75.240
	250N	1020	208CB	131.25
	250N	1020	2470	53.360
35	250CA	1020	217CE2	97.310
	250CA	1020	208CB	136.92
	250CA	1020	2470	57.350
	217CE2	1020	208CB	64.610
	217CE2	1020	2470	103.98
40	208CB	1020	2470	160.34
	206NH1	1021	206CD	63.610
	206NH1	1021	206CZ	23.320
	206NH1	1021	206NE	44.300
				500

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	206NH1	1021	2080G	119.29
	206NH1	1021	200NH2	93.260
	206CD	1021	206CZ	. 48.080
	206CD	1021	206NE	26.130
5	206CD	1021	2080G	59.000
	206CD	1021	200NH2	72.680
	206CZ	1021	206NE	23.690
	206CZ	1021	2080G	107.07
	206CZ	1021	200NH2	101.44
10	206NE	1021	2080G	84.290
	206NE	1021	200NH2	92.980
	. 2080G	1021	. 200NH2	52.780
	250CA	1022	247NE	114.53
	250CA	1022	2470	, 64.620
15	250CA	1022	247CZ	128.51
	250CA	1022	247CG	95.540
	250CA	1022	250C	23.580
	250CA	1022	247CD	114.32
	250CA	1022	250N	20.550
20	250CA	1022	247NH2	120.77
	250CA	1022	2500	37.250
	247NE	1022	2470	86.700
	247NE	1022	247CZ	21.230
	247NE	. 1022	247CG	43.200
25	247NE	1022	250C	91.090
	247NE	1022	247CD	22,540
	247NE	1022	250N	124.46
	247NE	1022	247NH2	37.560
	247NE	1022	2500	82.000
30	2470	1022	247CZ	107.10
	2470	1022	247CG	44.460
	2470	1022	250C	57.580
	2470	1022	247CD	68.380
	2470	1022	250N	52.860
35	2470	1022	247NH2	123.53
	2470	1022	2500	41.550
	247CZ	1022	247CG	62.780
	247CZ	1022	250C	106.76
	247CZ	1022	247CD	39.430
40	247CZ	1022	250N	143.24
	247CZ	1022	247NH2	20.530
	247CZ	1022	2500	
	247CG	1022	250C	75.970
				501

	WO 03/048733				
	247CG	•	1022	247CD	24.070
	247CG		1022	250N	92.820
	247CG		1022	247NH2	80.760
	247CG	• •	1022	2500	58.790
5	250C		1022	247CD	91.780
	250C		1022	250N	37.390
	250C		1022	247NH2	104.02
	250C	1	1022	2500	18.310
	247CD		1022	250N	115.79
10	247CD		1022	247NH2	58.770
	247CD		1022	2500	77.290
-	250N		1022	247NH2	140.47
	250N		1022	2500	42.510
	247NH2		1022	2500	105.05
15			•		

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WHAT IS CLAIMED IS:

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- 1. A composition comprising a UPPS in crystalline form.
- 2. The composition according to claim 1 wherein said UPPS is a dimer.
- 3. The composition of claim 1 wherein said UPPS is a Streptococcus pneumoniae UPPS.
- 4. The composition according to claim 1 comprising a protein wherein defined by coordinates of Table IA, interatomic distances in Table ΠA, or angles of active site residues listed in Table IIIA, in an essentially pure native form or a homolog thereof.
- 5. A prenyltransferase of claim 4 which is in its native crystalline form.
 - 6. A prenyltransferase according to claims 4 or 5 wherein said prenyltransferase has an active site formed by the amino acids Arg247, Gly250, Arg206, Arg200, Ser208, Tyr217, Asp28, Tyr70, Ile26, Phe72, Asn76, Met27, Ala71 as ligands to IPP.
- 7. A prenyltransferase according to claims 4 or 5 wherein said prenyltransferase has an active site formed by the amino acids Asp28-Arg32, Arg79, Met27, His45, Gly48, Met49, Leu52, Ala71, Tyr70, Leu90, Pro91, Phe94, Phe149 as ligands to FPP.
 - 8. A composition comprising the prenyltransferase of claim 4 in complex with the substrate FPP wherein defined by coordinates of Table IB, interatomic distances in Table IIB, or angles of active site residues listed in Table IIIB.
 - 9. A composition comprising the prenyltransferase of claim 4 in complex with the substrate IPP wherein defined by coordinates of Table IC, interatomic distances in Table IIC, or angles of active site residues listed in Table IIICB.
- 25 10. A heavy atom derivative of a *Streptococcus pneumoniae* UPPS crystal wherein the prenyltransferase comprises a protein having the coordinates listed in Tables IA-IC, IIA-IIC, or IIIA-IIIC.
 - 11. A prenyltransferase according to claim 4 wherein said prenyltransferase is characterized by an $\alpha+\beta$ fold with three layers, $\alpha\beta\alpha$, wherein the β -strands form a six-strand parallel β -sheet and three α -helices pack against one face of the sheet and three to four α -helices located on the opposite face.

12. A composition comprising a *Streptococcus pneumoniae* UPPS in orthorhombic crystalline form having a space group of P2₁2₁2₁.

- 13. The composition according to claim 12 wherein the crystalline form has lattice constants of a = 59.6Å, b = 118.0Å, c = 178.2Å.
- 5 14. The composition according to claim 12 wherein the crystalline form contains two 60 kDa dimers in an asymmetric unit.
 - 15. A composition comprising a *Streptococcus pneumoniae* UPPS in orthorhombic crystalline form having a space group of I2₁2₁2₁.
- 16. A composition comprising a co-crystal of Streptococcus pneumoniae UPPS
 in complex with a substrate IPP in orthorhombic crystalline form having a space group selected from the group consisting of P2₁2₁2₁ and I2₁2₁2₁.
 - 17. A composition comprising a co-crystal of *Streptococcus pneumoniae* UPPS in complex with a substrate FPP in monoclinic crystalline form having a space group of P2₁.
- 18. The composition according to claim 17 wherein the crystalline form has lattice constants of a= 58.1 Å, b = 44.6 Å, c = 115.5Å, β = 98.7°.

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- 19. A process for determining a crystal structure form using the structural coordinates of a *Streptococcus pneumoniae* UPPS crystal or portions thereof, to determine a crystal form of a mutant, homologue, or co-complex of a binding pocket or active site by molecular replacement.
- 20. A process of identifying an inhibitor compound capable of binding to and inhibiting the enzymatic activity of a *Streptococcus pneumoniae* UPPS said process comprising:
- a) introducing into a suitable computer program information defining an active
 25 site conformation of a UPPS molecule comprising a conformation defined by the coordinates and listed in Table IA, IIA, or IIIA wherein said program displays the three-dimensional structure thereof;
 - b) creating a three dimensional structure of a test compound in said computer program;
- c) displaying and superimposing a model of said test compound on a model of said active site;

d) incorporating said test compound in a biological prenyltransferase activity assay for a prenyltransferase characterized by said active site; and

- e) determining whether said test compound inhibits enzymatic activity in said assay.
- 5 21. A process designing drugs useful for inhibiting UPPS activity using the atomic coordinates of a *Streptococcus pneumoniae* UPPS crystal to computationally evaluate a chemical entity for associating with a active site of a UPPS enzyme.
 - 22. A method of modifying a test UPPS polypeptide comprising:
- a) providing a test UPPS polypeptide sequence having a characteristic that is
 targeted for modification;
 - b) aligning the test UPPS polypeptide sequence with at least one reference UPPS polypeptide sequence for which an X-ray structure is available, wherein the at least one reference UPPS polypeptide sequence has a characteristic that is desired for the test UPPS polypeptide;
- c) building a three-dimensional model for the test UPPS polypeptide using the three-dimensional coordinates of the X-ray structure(s) of the at least one reference UPPS polypeptide and its sequence alignment with the test UPPS polypeptide sequence;
 - d) examining the three-dimensional model of the test UPPS polypeptide for a difference in an amino acid residue as compared to the at least one reference polypeptide, wherein the residues are associated with the desired characteristic; and

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- e) mutating an amino acid residue in the test UPPS polypeptide sequence located at a difference identified in step (d) to a residue associated with the desired characteristic, whereby the test UPPS polypeptide is modified.
- 23. A process of identifying an inhibitor compound capable of inhibiting the enzymatic activity of a *Streptococcus pneumoniae* UPPS according to claim 4, said process comprising:
 - a) carrying out an *in vitro* assay by introducing said compound in a biological prenyltransferase activity assay containing a prenyltransferase according to claim 4; and
 - b) determining whether said test compound inhibits the enzymatic activity of the prenyltransferase in said assay.

24. A product of the process of claim 20 or 23 which is a peptide, peptidomimetic, or synthetic molecule and is useful for inhibiting a metallo-beta lactamase in treatment of bacterial infections in a mammal.

- 25. A product according to claim 24 wherein said product is a competitive or non-competitive inhibitor of the *Streptococcus pneumoniae* prenyltransferase.
- 26. A process designing drugs useful for inhibiting *Streptococcus pneumoniae* UPPS comprising using the atomic coordinates of a *Streptococcus pneumoniae* UPPS crystal or the atomic coordinates of a *Streptococcus pneumoniae* UPPS in complex with FPP or IPP to computationally evaluate a chemical entity for associating with the active site of a *Streptococcus pneumoniae* UPPS.

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- 27. The process according to claim 26 comprising the step of using the structure coordinates of *Streptococcus pneumoniae* UPPS to identify an intermediate in a chemical reaction between a prenyltransferase and a compound that is a substrate or inhibitor of said prenyltransferase.
- 28. The process according to claims 26 or 27 wherein said structure coordinates comprise the coordinates listed in Tables IA-IC, IIA-IIC, or IIIA-IIIC.

Figure 1A

Figure 1B

Figure 2A

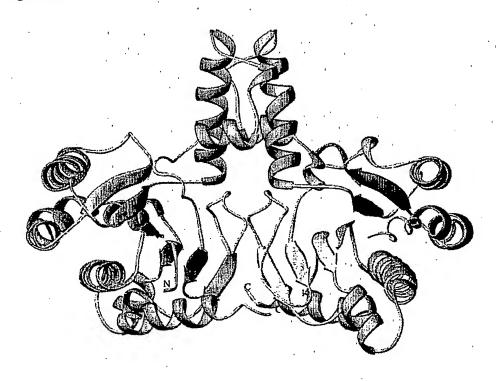


Figure 2B

UPS (S. pneumoniae)

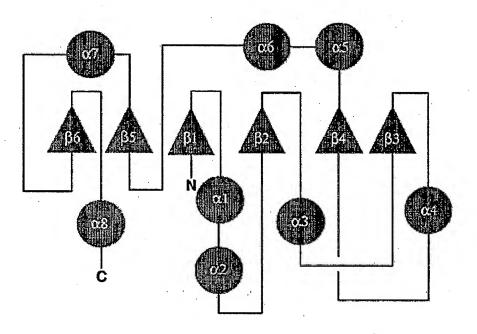


Figure 3A

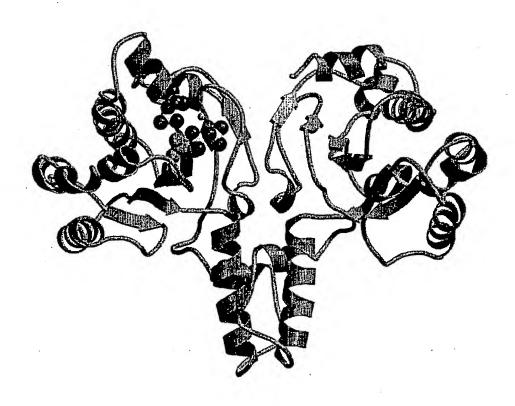


Figure 3B

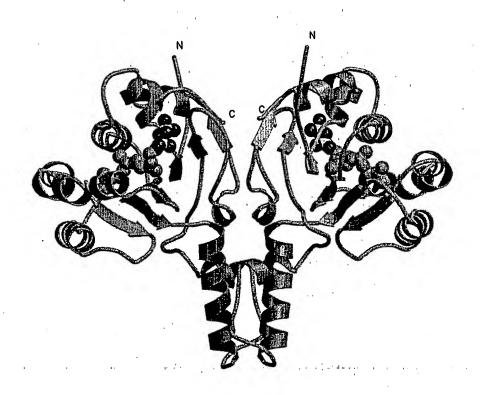


Figure 4A

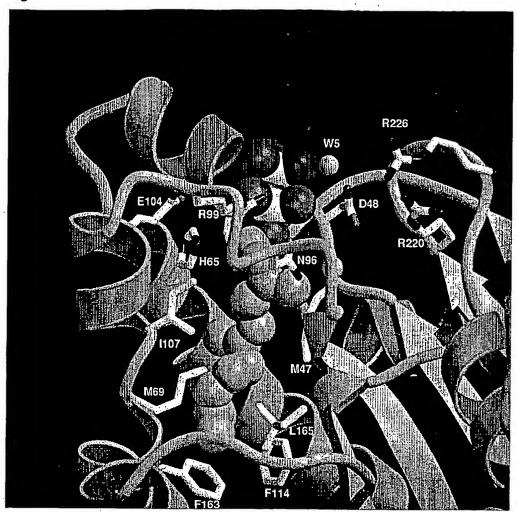
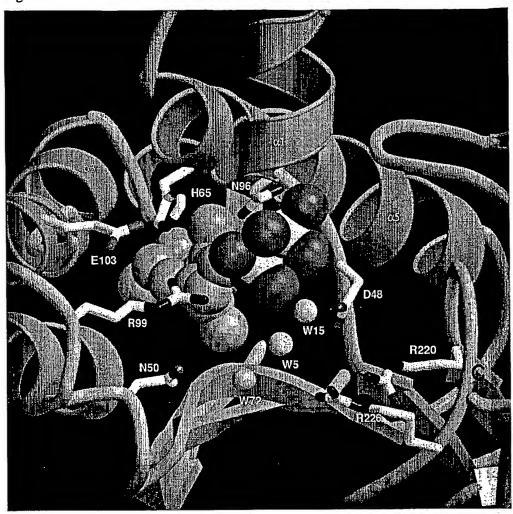
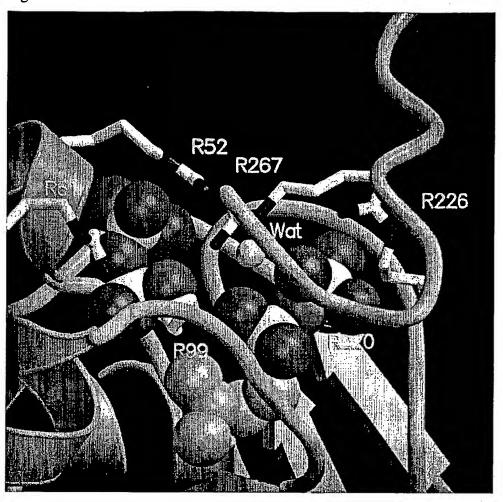


Figure 4B



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Figure 5



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698917InventoryList.txt

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"PCT/US02/38715"

"20 Dec 2002"

"1. DOE0901 Notification of Status of Requirements Under 35 U.S.C. 371"

"2. ISA202 Notification of Receipt of Search Copy"

"3. ISA225 Inv to Furnish Nucleotide and/or Amino Acid Seq Listing Complying with Standard"

"4. RO101 PCT/RO/101 Form Record Copy"

"5. RO101S PCT/RO/101 FORM SEARCH COPY"

"6. RO102N Notification concerning Payment of Prescribed Fees-No R eply"

"7. RO105 Notification of The International Application # and of the Intl. Filing Date"

"8. RO106 Invitation To Correct Defects in The International Application (Incl. Annex ABC)"